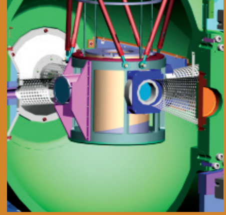
LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

NOVEMBER 2010



1663

NEARLY
A TRILLION
MICROORGANISMS
LIVE IN THIS
AMOUNT
OF
SOIL

What are they doing,
and what could they be doing for us?

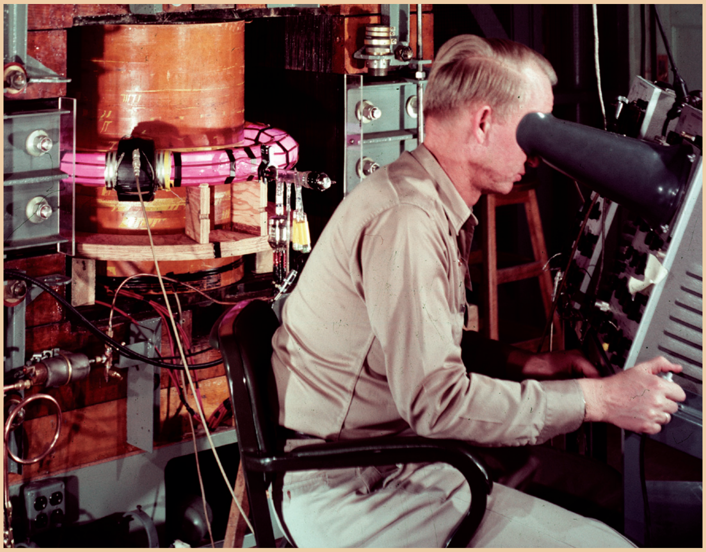
Los Alamos
NATIONAL LABORATORY
EST. 1943

1663

About Our Name: During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo: Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo will appear at the end of the article.

About the Cover: Microorganisms in the soil perform services that are essential to the survival of all plant and animal life on Earth, and learning to harness their abilities could lead to revolutionary new technologies in agriculture, medicine, environmental management, and more. However, only about 1 percent of these microorganisms are understood by science today. Can we rapidly learn about the other 99 percent?


LOS ALAMOS ARCHIVE

1952: Los Alamos scientist Jim Tuck with the "Perhapsatron," a device he designed to slowly compress a hot plasma to nuclear fusion conditions by using magnetic fields.

My View

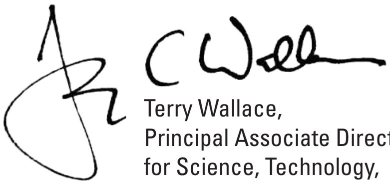
Vibrant Science

The scientific and technological problems facing our country today are both diverse and complex, and addressing them requires highly innovative, multidisciplinary research. Bringing talented scientists from many fields to our facilities and laboratories is therefore critical to our mission, but it is only part of what we must do to meet our national responsibility. More broadly, we must sustain an environment of collaboration that encourages the best and brightest minds to do their most exceptional thinking. In short, we must remain committed to the vibrancy of our science.

Vibrant science is vigorous, energetic, and broad—as it must be, if it is to confront complex, interconnected challenges. Consider, for example, the burning of fossil fuels and the resulting rise in atmospheric carbon emissions. These pose serious security concerns—in terms of our energy supply, our economy, our natural environment, and our exposure to geopolitical instability spawned by shifting natural resource patterns. These are problems whose solutions necessarily span many disciplines, requiring a tremendous range of scientific research.

This issue of 1663 highlights several multidisciplinary approaches to the carbon problem. For example, you'll read about a unique collaboration to create a "smart" power grid to accommodate an increasing deployment of renewable energy instead of carbon-emitting sources. You'll read about a novel program to examine the microscopic life found in the earth beneath our feet and how that life affects the global carbon cycle. You'll read about efforts to improve the manufacturability of carbon-free fuel cells, and plans to modify an enzyme to grow renewable biofuels and mitigate carbon emissions from power plants. All of these lines of research (and many others!) are needed to address the broader carbon challenge.

Los Alamos is producing world-leading science on many fronts, and the ability to connect fundamental discoveries to real-world applications is a hallmark of our success. Both the discoveries and the applications emerge from vibrant research that relies on the variety of expertise and capability gathered in common purpose here at Los Alamos.



Terry Wallace,
Principal Associate Director
for Science, Technology,
and Engineering

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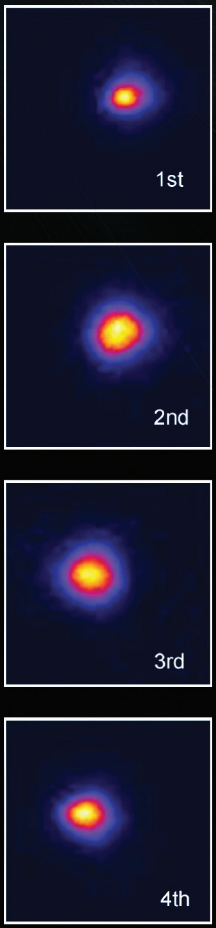
Dynamic Vision

In a series of crucial experiments, DARHT proves it's ready to become the workhorse facility of the nuclear weapons community.



The images (right) show the four electron pulses generated when DARHT's second axis fires. When run through a foil, they create a train of four x-ray pulses, depicted here as white spots in a purple ether (facing page). Together with a lone pulse (left) from DARHT's first axis, the intense x-rays are used to penetrate and image an exploding object (above).

November, 2009. Wendy Vogan McNeil stood in the control room of the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility as the machine operators began their countdown for experiment H3837. McNeil and fellow experimenters Matthew Briggs and Lawrence Hull had spent about 10 months preparing for this moment. They had chosen the target material—a newly developed alloy—and had it fashioned into a miniature hockey puck that McNeil later set atop 31 grams of high explosive. They calculated that once the explosive detonated, it would take about 8 millionths of a second (8 microseconds) for a shock wave to reach the puck, rush through it, and begin to blow the top surface off. A computer simulation predicted how much the alloy would be compressed by the shock wave's passing, and helped them determine when DARHT's two x-ray sources—it's dual axes—should fire to take the radiographs (x-ray images) that would capture the compression in action.

Now, before McNeil could take a breath or cross her fingers for luck, both sources fired, and the experiment was over.

McNeil waited for the radiographs to appear on the control-room monitors. She would process each image and measure the density of the alloy directly behind the shock-wave front. Briggs, meanwhile, would process velocimetry data to measure how fast the puck's top surface moved. (See figure on page 7.) Together, the two measurements would constrain theoretical models of how the new alloy responds to being shocked. Because the best models would be incorporated into the enormous computer codes that aim to predict the long-term behavior of the nation's nuclear weapons, the measurements were of interest to several of the Laboratory's materials and physics groups.

More people, however, were interested in whether DARHT's second axis had operated successfully in multipulse mode, that is, if it had fired off four high-intensity, well-defined x-ray pulses in a precisely timed sequence totaling less than 1.6 microseconds. Various beam diagnostics would tell that story to DARHT's machine diagnostics crew.

But the major story concerned the timing of DARHT's two axes. DARHT was designed to radiograph a target from two vantage points simultaneously. That's why the two axes are set perpendicular to each other, so that x-rays from the first axis can illuminate the target from the front, say, at the same time that one of the second-axis pulses hits it from the side. Nearly everyone wanted to know if the fifth radiograph—the one from the first axis—lined up with the third pulse from the second axis.

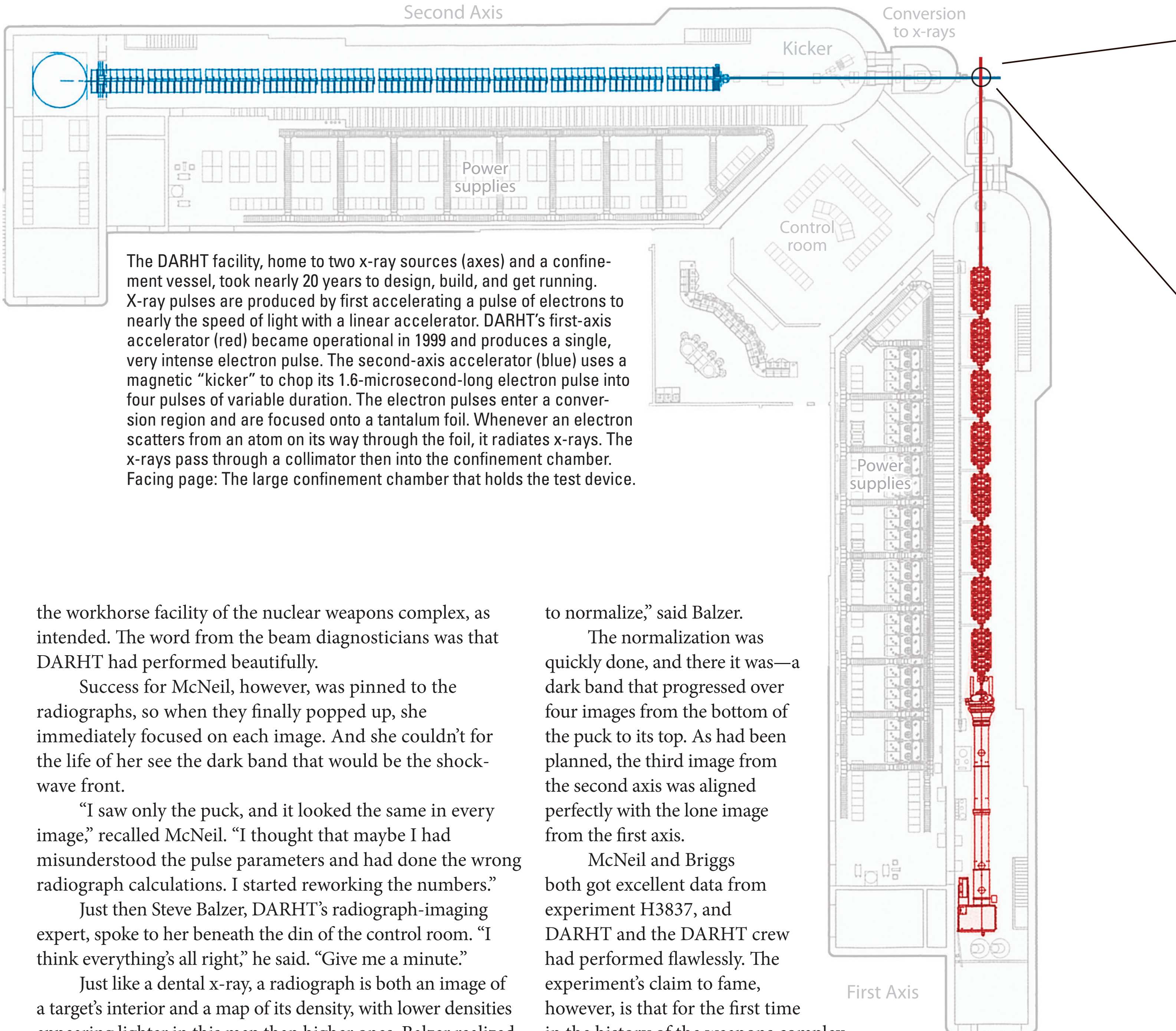
Subrata Nath, a group leader in the Weapons Experiments (WX) Division and DARHT's principal accelerator physicist, had a stake in how well the two sources performed. A few years back, when prospects for the second axis were grim, Nath (then deputy project director) was one of the principal architects of a plan to revive it. He knew that for the many people who had followed DARHT's progress over the years, experiment H3837 was a litmus test.

In the big picture of the nuclear weapons community, a sequential set of sharp, clear radiographs would help scientists understand the dynamic interactions between a shock wave and a target far better than would a single radiograph. One of the goals of H3837 was to demonstrate that the second axis could generate the intense x-ray pulses needed to produce four clean images. As for the pair of radiographs taken from different vantage points, if the pulses fired at the right time, scientists could take the two radiographs and do a three-dimensional reconstruction of the target to see if the shock wave compressed it as desired. Thus, another goal was to check the relative timing between the axes.

If something went wrong with either of DARHT's x-ray sources (and the sources are so complicated there's always the possibility of *something* going wrong), Nath would be one of the people who would decide if the problem was serious enough to cancel the next experiment, already scheduled for early December. That experiment was to be a so-called hydrotest, conducted on a full-scale mock nuclear warhead, and would be a live run of the events that trigger a nuclear explosion. McNeil's alloy-puck experiment notwithstanding, the primary motivation behind experiment H3837 was to demonstrate that DARHT was ready to conduct December's hydrotest.

A Good Day

Both the multipulse and 3-D capabilities needed to be working well and reliably if DARHT were to become



The DARHT facility, home to two x-ray sources (axes) and a confinement vessel, took nearly 20 years to design, build, and get running. X-ray pulses are produced by first accelerating a pulse of electrons to nearly the speed of light with a linear accelerator. DARHT's first-axis accelerator (red) became operational in 1999 and produces a single, very intense electron pulse. The second-axis accelerator (blue) uses a magnetic "kicker" to chop its 1.6-microsecond-long electron pulse into four pulses of variable duration. The electron pulses enter a conversion region and are focused onto a tantalum foil. Whenever an electron scatters from an atom on its way through the foil, it radiates x-rays. The x-rays pass through a collimator then into the confinement chamber. Facing page: The large confinement chamber that holds the test device.

the workhorse facility of the nuclear weapons complex, as intended. The word from the beam diagnosticians was that DARHT had performed beautifully.

Success for McNeil, however, was pinned to the radiographs, so when they finally popped up, she immediately focused on each image. And she couldn't for the life of her see the dark band that would be the shock-wave front.

"I saw only the puck, and it looked the same in every image," recalled McNeil. "I thought that maybe I had misunderstood the pulse parameters and had done the wrong radiograph calculations. I started reworking the numbers."

Just then Steve Balzer, DARHT's radiograph-imaging expert, spoke to her beneath the din of the control room. "I think everything's all right," he said. "Give me a minute."

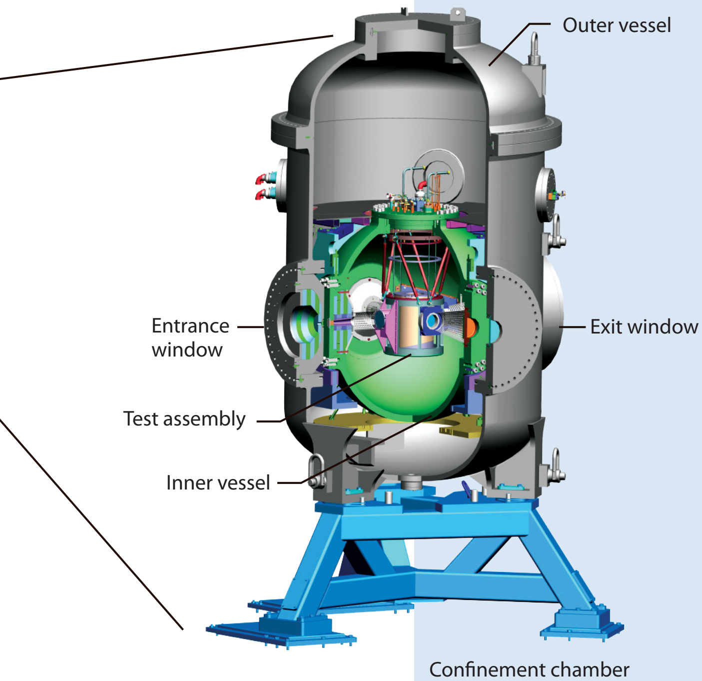
Just like a dental x-ray, a radiograph is both an image of a target's interior and a map of its density, with lower densities appearing lighter in this map than higher ones. Balzer realized that there wasn't much high explosive under the puck, so the shock wave was relatively weak, and increased the alloy's density by only a few percent. Uncompressed material in front of the shock wave looked about the same as the compressed material behind it. The shock wave could be made much more noticeable if the puck's density range coincided with the radiograph's gray scale. This could be achieved by removing from each pixel a "background" component corresponding to x-rays transmitted by the unshocked material. "We just needed to normalize," said Balzer.

The normalization was quickly done, and there it was—a dark band that progressed over four images from the bottom of the puck to its top. As had been planned, the third image from the second axis was aligned perfectly with the lone image from the first axis.

McNeil and Briggs both got excellent data from experiment H3837, and DARHT and the DARHT crew had performed flawlessly. The experiment's claim to fame, however, is that for the first time in the history of the weapons complex, a four-frame x-ray "movie" had been made of an exploding object while at the same time another radiograph had captured the action from a different vantage point.

An Inside Look

No matter what its other accomplishments turn out to be, DARHT must provide scientists with a view inside a mock nuclear warhead during a hydrotest. The heart of a nuclear warhead, its "primary," is essentially a hollow shell of



Confinement

"Prior to 2007, experiments at DARHT were executed outside in the open air. The explosive shots were often spectacular, thrilling events, but they were also very loud, and the shot setup and cleanup were long, complicated, and expensive processes. Sometimes it would take weeks to clean up the firing site and the surrounding area. And while measures were taken to mitigate impacts to the environment, there were limits to what was possible.

"So in 2007 DARHT was reconfigured to use a confinement system. The test device is now placed in a hexapod alignment fixture [central can in the illustration] that can be positioned to sit precisely at the intersection point of the two pulsed x-ray beams. The hexapod is surrounded by a thick-walled steel vessel [green], which is surrounded by another thick-walled steel cylinder [gray]. Now, when the explosion goes off, it is completely confined. You hear virtually nothing, just a deep "pong," like someone hitting the bottom of a cooking pan with a big spoon. The thrill is also gone, but we made a commitment to the environment and we've stood by it."

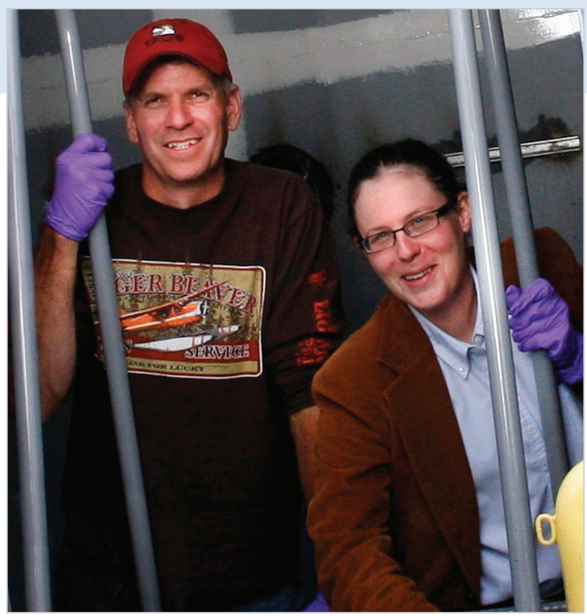
—Dennis Royer, DARHT firing site coordinator

plutonium surrounded by a thick rind of high explosives. In a mock warhead, the primary's plutonium shell is replaced with a surrogate—a shell of highly dense, "dead" material such as depleted uranium.

The test of a mock warhead is called a hydrotest because once the high explosives that surround the surrogate primary are detonated, a shock wave races inward at supersonic speeds, smacks into the hollow shell, and liquefies it on impact. It is then a problem in hydrodynamics to understand in detail what happens as the shell implodes, that is, as the liquid is driven inward at high speed and compressed intensely into a compact sphere.

In a real weapon, with a plutonium primary, the sphere would be bombarded with neutrons, which would initiate a fission chain reaction, ultimately leading to a nuclear explosion. With the surrogate primary, there is no fission and none of the accompanying radiation; the chemical explosion simply consumes the mock warhead and the hydrotest ends.

DARHT is currently the only facility in the world that produces x-ray pulses with enough energy and intensity to pass through the dense, depleted uranium shell in the mock warhead and take a radiograph. DARHT is also the only facility that can produce those pulses fast enough to capture the details of the implosion, to make a four-frame movie, and to allow for a 3-D reconstruction. That's why DARHT



Dennis Royer (left) and Wendy Vogan McNeil inside an enclosure sitting atop the confinement chamber.

is considered to be such a remarkable facility and one of the crown jewels of the nuclear weapons community.

"It was not an easy task to build this facility," says Nath. "Consider coordinating the pulses from the first and second axes. We have to be able to customize the duration of each pulse coming from the second axis. The two accelerators have to run independently of one another, yet in the end their respective x-ray pulses have to hit the target within a few nanoseconds of each other."

Many scientists were skeptical that such exquisite timing could be achieved. Indeed, before McNeil's experiment, it had never been attempted on an exploding target. But the scientists, engineers, and technicians from the Los Alamos, Lawrence Livermore, and Lawrence Berkeley national laboratories who designed and built DARHT knew it could be done.

"The real challenge is that we have one chance to do everything right," says Nath. "Each accelerator has hundreds of triggers that have to fire in the right sequence to produce the x-ray pulses, and if any fail, the experiment is lost. But we've been able to overcome this and many more challenges because of the genuine partnership between the three laboratories. It's been the best collaboration I've seen."

Assurance without Testing

The United States stopped testing nuclear weapons in 1992, a decision that deprived weapons scientists of a means to obtain information about how warheads age, what their lifespan is, and whether refurbishing a device would introduce enough small changes to turn the world's most powerful weapons into duds.

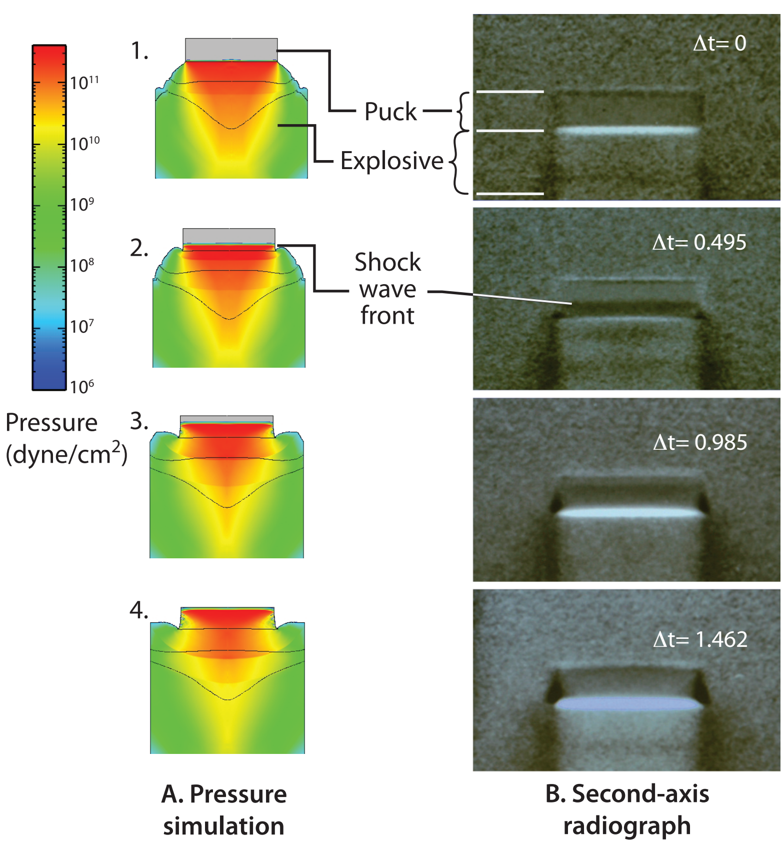
The Deparatment of Energy supported the testing moratorium by sponsoring the massive Stockpile Stewardship program, which uses a combination of weapons surveillance (weapons are removed from the stockpile, disassembled, and inspected for mechanical problems), computer simulations of the moment-by-moment performance of an exploding nuclear weapon, and nonnuclear tests of warheads and their components to ensure that the stockpile remains reliable and safe.

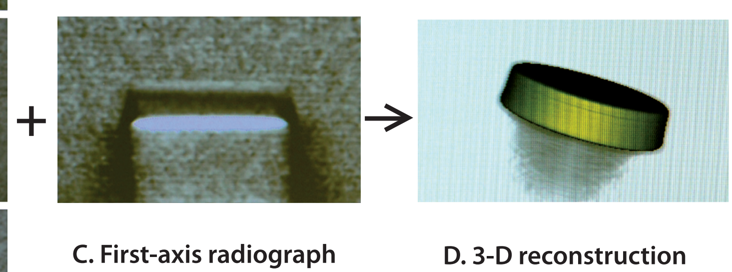
Numerous physics models, including those describing nonlinear processes and a material's response to shock waves, go into the computer simulations, which are among the most complex in the world. It's not by accident, then, that Los Alamos is home to the world's fastest computers.

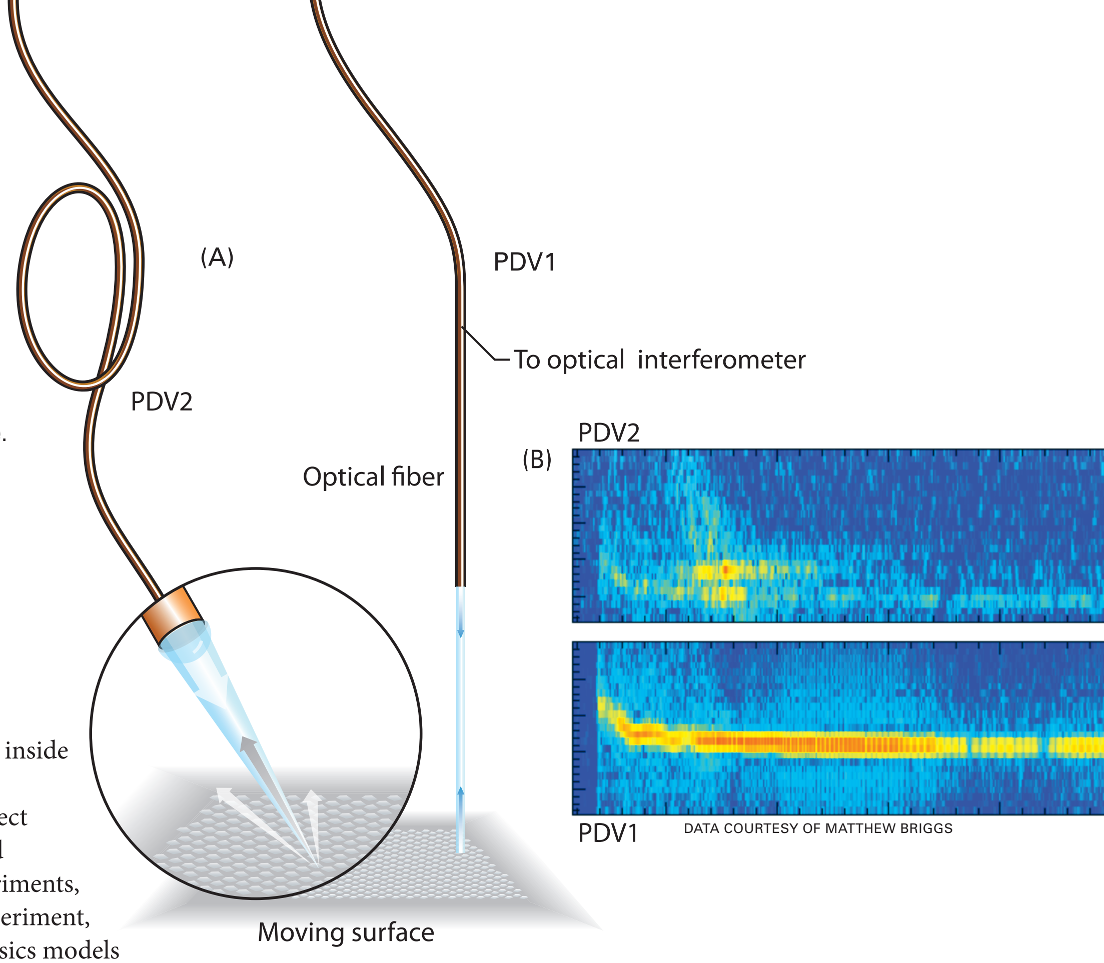
The simulations are benchmarked against results from past weapons tests, but their predictions about what

(A) As seen in these simulations of experiment H3837, the detonation of high explosives beneath the target (an alloy puck) launches an extreme high-pressure wave (shock wave) that traverses the quarter-inch-thick puck in about 1.4 microseconds. The pressure behind the wave front is sufficient to compress the alloy and increase its density. (B) X-ray pulses from DARHT's second axis are generated so fast that they "freeze frame" the shock wave. Each pulse generates a radiograph that records the intensity of x-rays transmitted through the target. Because denser regions attenuate x-rays more, the radiographs yield density information. (C) In H3837 the first-axis radiograph coincided perfectly with the second-axis' third radiograph. Scientists use the two perspectives to check the symmetry of an implosion. (D) Tomographic software can construct a 3-D model of the target.

RADIOGRAPHS COURTESY OF S. BALZER, PRESSURE CALCULATIONS COURTESY OF K. KWIATKOWSKI, AND 3-D PROJECTIONS COURTESY OF J. HARSH



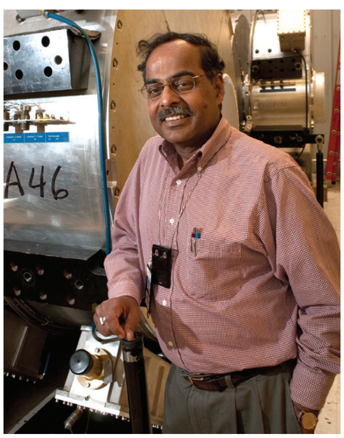




Photon Doppler velocimetry (PDV) is used to resolve the speed and direction of the top surface of the puck. (A) Light from an optical fiber is focused onto the target's surface. Some of the light reflects right back into the fiber. The fiber is one arm of a Michelson interferometer, and as the surface moves, the interferometer reveals its speed. Several fibers placed at angles to the surface yield the direction. (B) The velocity as a function of time from two PDV fibers.

happens to materials after years inside a radioactive warhead, or about how manufacturing changes affect the weapon's performance, need confirmation. Small-scale experiments, such as McNeil's alloy-puck experiment, provide data to validate the physics models that account for those changes.

But the ultimate test of a simulation is a comparison of its results with the results of a hydrotest, especially concerning how the primary performs. In a modern nuclear device, if the primary underperforms, the so-called "secondary," which generates the bulk of the nuclear explosion, won't ignite. The device fizzles.



Subrata Nath

Thus, when given the correct command sequence, primaries must detonate with 100 percent reliability, but they must not detonate or produce a nuclear explosion if accidentally jostled, dropped, hit with a hammer, set afire, or subjected to one of a thousand other unplanned actions. In one sense, for safety's sake, primaries are predisposed to fail, and even minute changes to their parts or materials—planned or unplanned—may cause them to do so. The only way to know for sure that a change is okay is to run a hydrotest, and DARHT is the only direct tool for conducting that test.

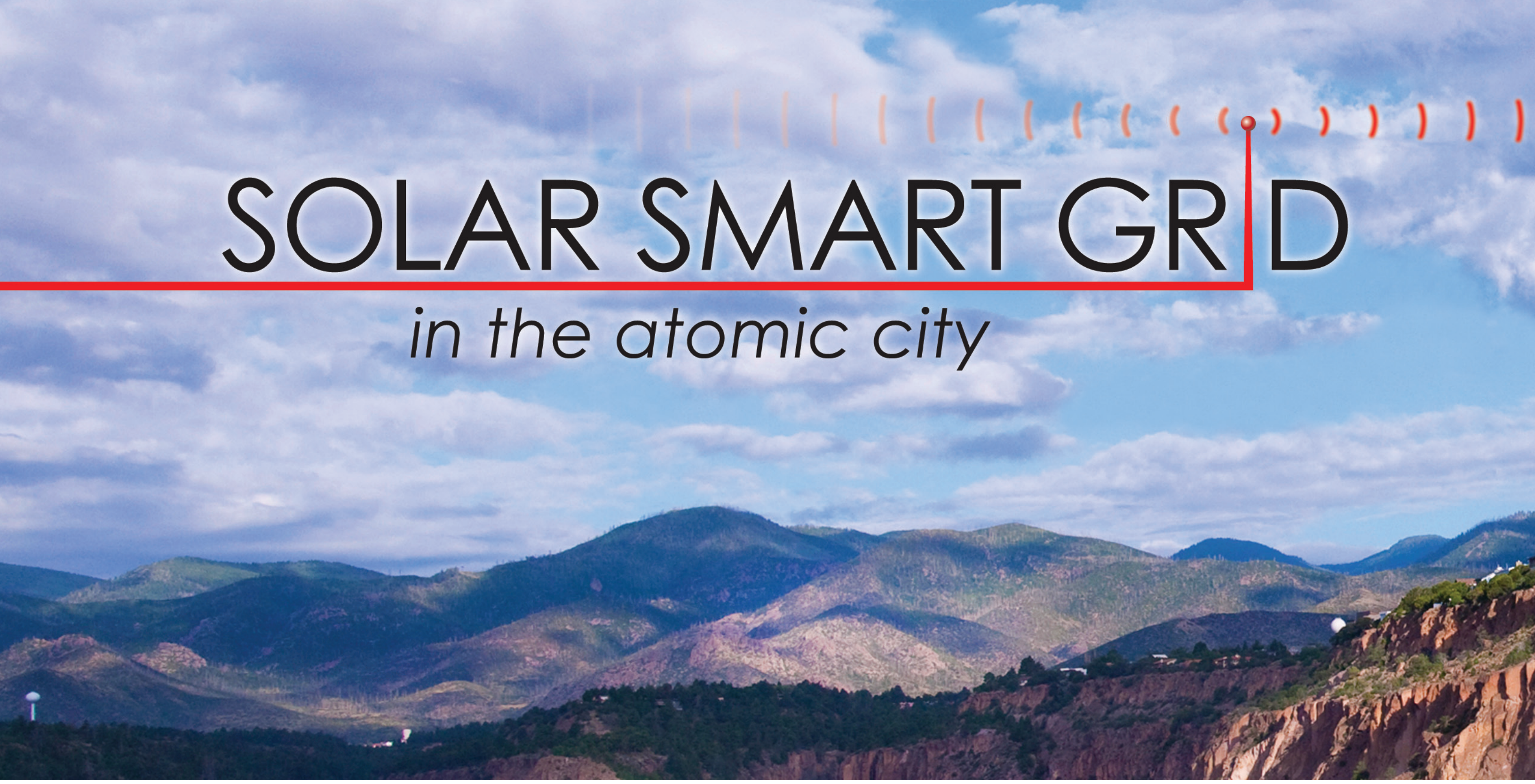
The Payoff

Early December 2009 found everyone associated with DARHT preparing for the full-scale hydrotest. It was hoped that the test would find the cause of an anomaly discovered earlier, because even a hint of uncertainty would cast a shadow on the safety, security, and reliability of the stockpile. On the big day, both axes were producing pulses that surpassed their design specifications. The test went flawlessly and helped put the anomalous issue to rest.

Of late, DARHT seems to prove its worth with every test, hydro or otherwise. In a recent experiment, the science staff members were baffled by what they saw in the first of four radiographs but then saw in the image sequence that the test object evolved as expected. The only thing wrong was the scientists' initial expectations. If the first radiograph had been the only one available, it would have generated hundreds of hours of discussion, endless emails, and a potentially costly experimental program to reproduce and understand the event. DARHT's multiple images made the whole further-investigation moot.

Helping to maintain a nuclear stockpile—and saving the taxpayers money. Now that's something you don't hear about every day. ❖

—Jay Schecker



SOLAR SMART GRID

in the atomic city

Los Alamos National Laboratory is known for interdisciplinary research. Still it's unusual to find a research project in which the Laboratory's Utilities Division leader (Andy Erickson) and a team of high-powered physicists and engineers will use their own workplace, the local Los Alamos County utility, the townspeople, and a foreign collaborator to help solve one of our nation's energy problems. The collaborator, Japan's New Energy and Industrial Technology Development Organization (NEDO), will be demonstrating how its technology could be part of the solution.

The problem—modernizing the nation's overburdened power grid—has captured the imagination of so many because there seems to be a "smart" solution, one that could transform our energy use as profoundly as cell phones and the Internet have transformed our communications. Called the smart grid, the solution involves consumers and smart meters in making the grid more cost effective, more compatible with renewable energy sources, and more resistant to blackouts. It's being tried on various scales across the nation.

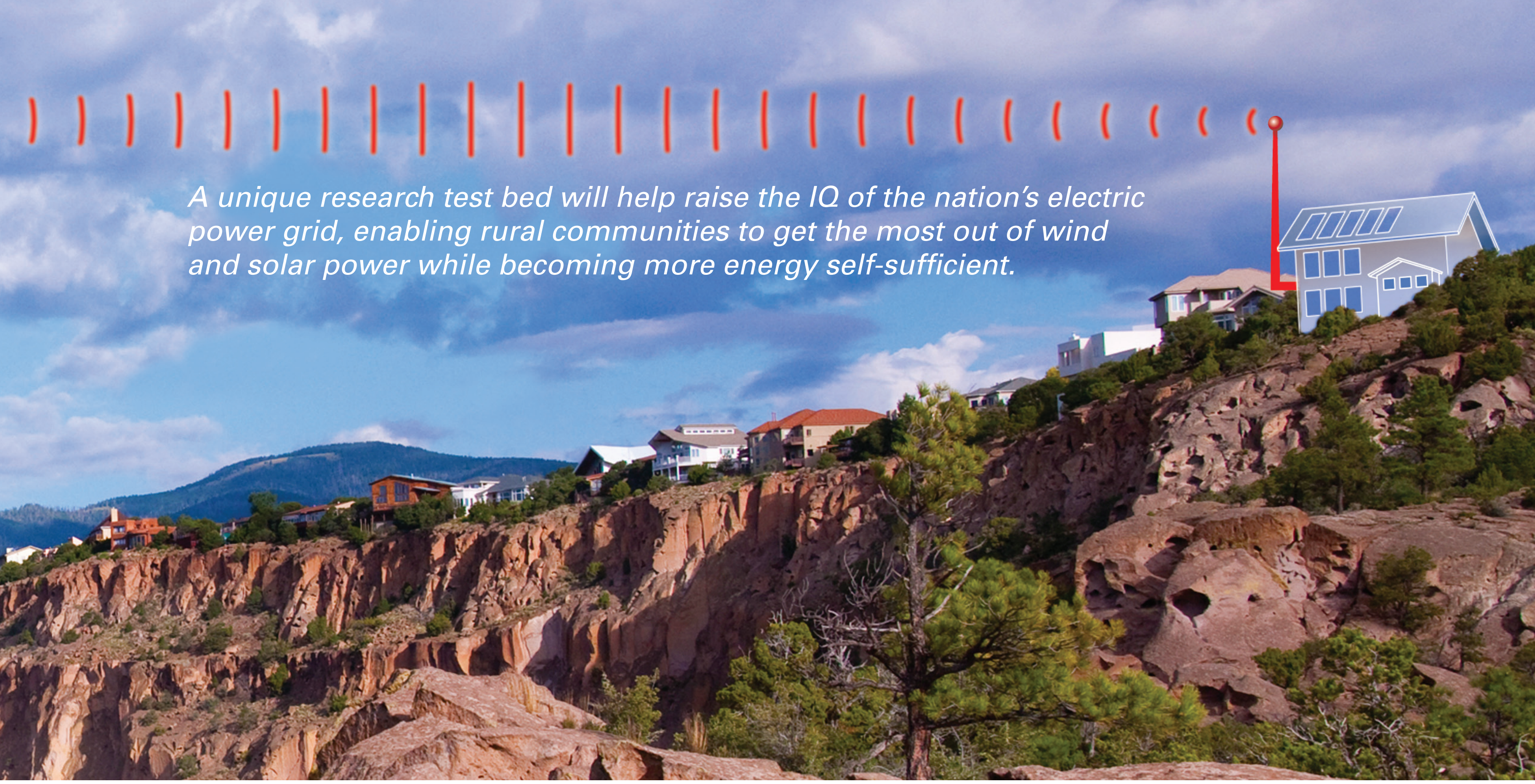
The Los Alamos-NEDO trial of a smart grid has a special focus: to help rural communities across the country incorporate renewable energy and smart grid technology in an affordable way. Erickson explains, "Our project is going to include computer simulation tools to help control, in real time, a community-scale smart grid demonstration that gets a significant amount of power from a large solar photovoltaic (PV) array. Based on the data we collect, we will design smart, cost-effective ways for small communities to incorporate renewables on their local grids."

What's Wrong with Today's Grid?

The nation was startled on August 14, 2003. Starting at 4:04 p.m. on a typical warm summer afternoon, the power went out in and around Akron, Ohio, and over the next seven minutes, the blackout rolled across most of the northeastern United States and Canada. At each successive failure, the grid tried to pick up the load, but line after line became overloaded, tripping breakers, shutting down generators, and causing town after town, state after state to go dark. The elevators, air conditioners, computers, electric clocks, commuter trains, airport monitors, street lights, office lights, radios, TVs, appliances, cash registers, the ticker tape at the New York stock exchange, the billboards on Times Square—almost every convenience of modern life—suddenly stopped working, and 50 million people were left to cope. It took days to recover, and business and personal losses totaled around $6 billion.

How could such a massive blackout occur? The reason stems from the properties of the grid. The North American electrical power grid is a system of four loosely connected, very large networks. Together they comprise about 3500 large power plants (mostly fossil fuel), interconnected by

Right: By volunteering to install smart meters (like the one shown here) in their homes and consider price signals when using electric power, Los Alamos residents can become part of the Los Alamos-NEDO smart grid project.



200,000 miles of high-voltage transmission lines connected in turn to millions of miles of low-voltage local distribution networks that deliver electricity on demand to about 131 million separate consumers. This system of centralized supply and distributed demand can produce up to 1 trillion watts of electric power continuously, electrifying virtually every building and facility in the United States and Canada.

The grid is an engineering marvel, but can be a bear to control when things go wrong. Unlike water or natural gas delivery systems, in which large water tanks or pressurized gas containers can store "product" for future delivery, there is little energy storage on today's grid. Thus, electrical energy must be consumed as soon as it's produced; supply and demand must be exquisitely balanced at all times. Because electrical energy travels over the lines at nearly the speed of light, the whole system acts like a single machine with nearly instantaneous feedbacks. That's why a series of accidental faults on the lines or operator errors or unexpected loads at times of peak demand can lead to an event like the 2003 rolling blackout. Even without massive blackouts, power outages and drops in voltage or power quality cause estimated business losses of $100 billion annually.

Because electricity must be consumed in real time and fossil-fuel power generation is much more controllable than consumer demand, demand is the tail that wags the dog in today's grid. Specifically, demand is forecast about 8 hours ahead of generation, affording time for "baseload" generation to be spun up to meet that demand. Typically, the predictions are sufficiently accurate to allow operators to control normal flows of power, and the difference is made up by buying and selling electricity every hour on the hour between utilities.

The system gets stressed during times of peak demand, for example, on hot summer days when all the air conditioners in the South or the West get turned on at nearly the same time. To meet that demand, the grid holds a certain amount of capacity in reserve: either coal-fired generators are operated below maximum power, which leads to high carbon emissions, or in a more expensive option, gas turbines are kept idle most of the time, ready to be spun up rapidly—in 15 minutes from a cold start—and put on line.

Finally, grid stability is seriously incompatible with the intermittent power from renewable energy sources. Solar irradiance and wind are fluctuating sources, and their power output can drop suddenly as clouds obscure the sun or the wind dies down. How do you keep the grid stable when suddenly a wind farm's contribution drops from 1700 megawatts to 300 megawatts in just a few minutes, as happened in Texas in 2008? How do you keep the voltage on the line from dropping, causing motors to burn out as they try to draw more and more current? And how do you manage to match supply to demand at every instant when there are hundreds or thousands of fluctuating solar and wind sources contributing a substantial fraction of the grid's power?

Loren Toole, a principal investigator in the Laboratory's part of the Los Alamos-NEDO smart grid project, recalls what happened in California in the 1980s: "When many wind

Above: The Los Alamos-NEDO smart grid project will incorporate two-way communication between the utility control system and digital smart meters. One will be installed in a NEDO smart house that will contain its own solar panels, smart appliances, and large storage battery.

John Arrowsmith (center) at the landfill site for the solar PV arrays with the Laboratory's Venkateswara Dasari and Carolyn Zerkle, both of whom were instrumental in starting the Los Alamos-NEDO project.

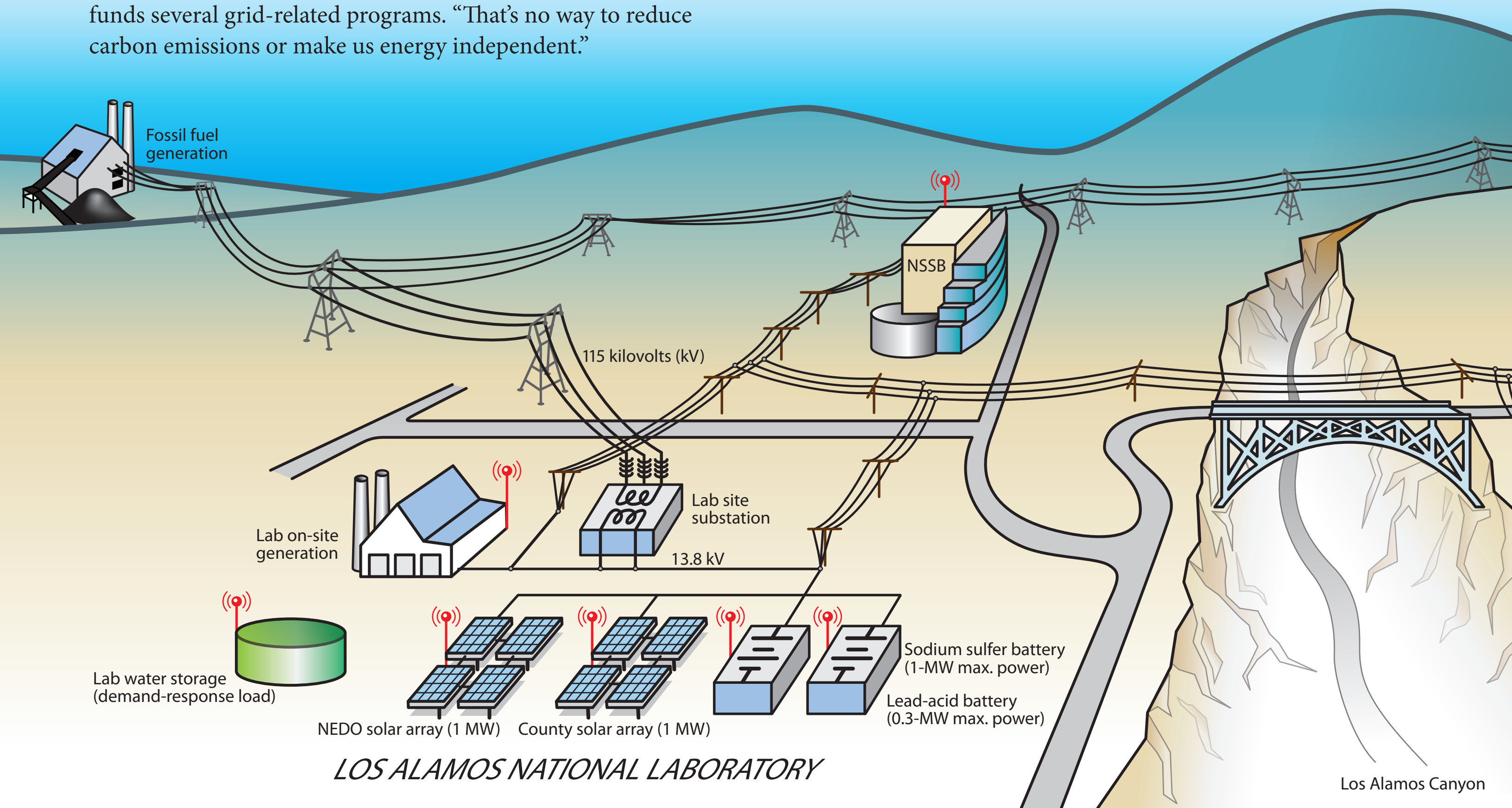
farms were incorporated into the grid over several years without proper controls and planning, a large fraction of the energy from wind farms had to be dumped before it ever reached the grid." The power was in excess of demand and would have destabilized the grid.

"Today, when renewable sources are added to the grid, they are being backed up by adding new fossil-fuel generating capacity. I liken that to driving with one foot on the accelerator and the other halfway on the brake," quips Karl Jonietz, the Laboratory's program manager for the Office of Electricity Delivery and Energy Reliability, which funds several grid-related programs. "That's no way to reduce carbon emissions or make us energy independent."

What Makes a Grid "Smart"?

Clearly, if renewables are to make a significant contribution to the nation's power grid in the next 20 years, the paradigm of grid operation has to change. No longer can demand be the tail that wags the dog. As supply becomes more distributed and less predictable, various means of storing energy have to be added to the grid, and demand has to be responsive to changes in supply. This requires building more intelligence into the grid at every level. And that intelligence can then be used to help solve all the grid's problems. So goes the argument for the smart grid, a set of concepts and technologies that emerged over several decades from interactions among industry, universities, and electric regulatory agencies. Today the Department of Energy is actively encouraging its implementation.

The present grid would become smart if it were given an overlay of information technology that could act, within each area, somewhat like a central nervous system. Digital two-way smart meters (the "nerves") would be located at points throughout the grid down to individual homes. Each meter would measure the state of the grid at its location—the amount of current flowing, the voltage values, and how far AC current deviates from its nominal (standard) value of 60 cycles per second—and send that data (using wireless communication, fiber optics, or other means) to the computerized utility control system (the "brain"). Each control system would input that data to its own predictive computer models that would forecast the future state of the local grid and recommend (to operators), or automatically implement, actions needed to maintain grid stability.



Those actions would include not just modifying power generation but also initiating a new paradigm: “demand response,” that is, getting users to change their demand in response to changes in supply. One approach to initiating demand response is the use of real-time price signals. Rates could be reduced during the night when demand is low and raised during times of peak demand or when the grid is stressed because of a failure in the system or a drop in output from renewables. Control systems would send price signals to smart meters, and those meters could be programmed by consumers to turn up the thermostats on hot afternoons when prices are high or turn off certain appliances, or delay the charging of electric cars, in order to reduce demand and help grid stability. In the smart grid revolution, consumers would be more informed and would have more control, either through their own energy management systems or through their local utility. By reducing levels of peak demand, consumers would help reduce the need for excess generating capacity, stresses on transmission lines, losses due to power disruptions, and so on.

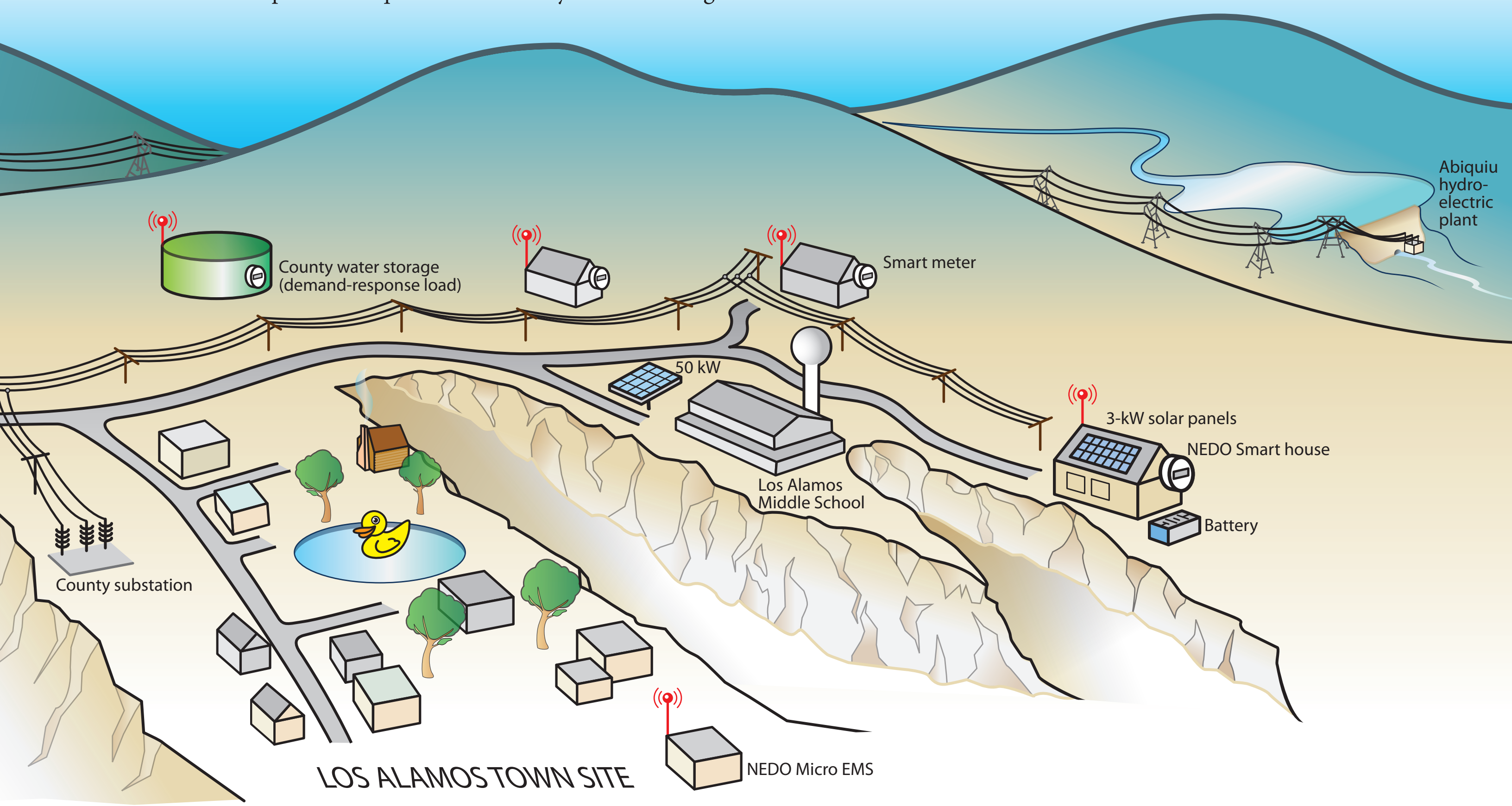
The individual pieces of technology—smart meters, smart appliances, communication systems—all exist, but integrating them into a working system, maintaining control over the system, getting the public to participate, and ensuring that the return on investment makes good business sense are objectives that are being explored in towns and cities across the nation.

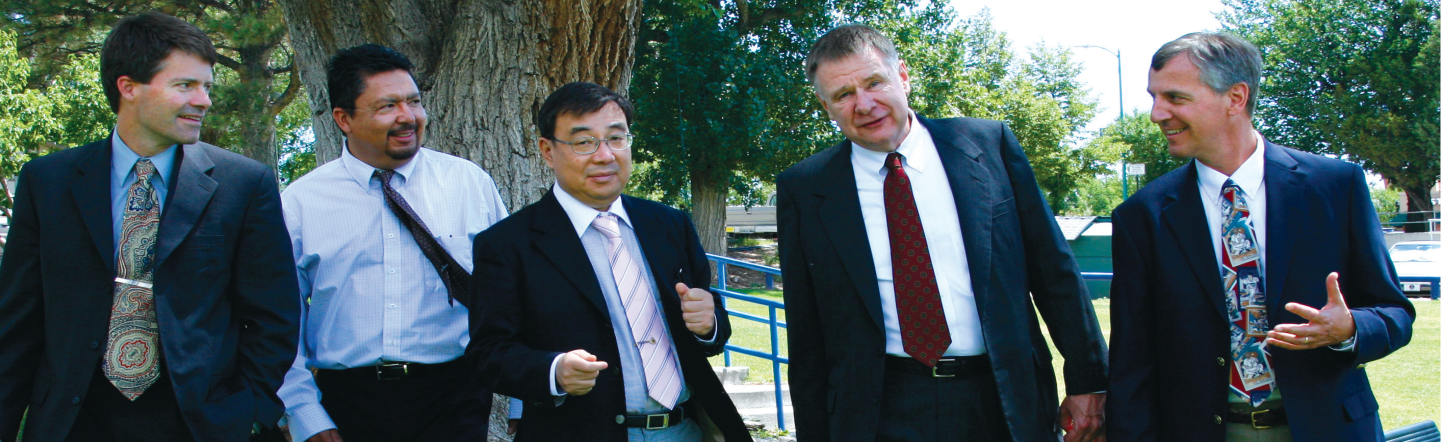
Los Alamos Gets Involved

The Los Alamos-NEDO smart grid project hopes to answer a particular question: how do you use smart grid technology to incorporate renewables at the community level? Jonietz explains, “Not all homeowners can afford to invest in solar panels, but often it’s feasible for local utilities to invest in large solar arrays that serve clusters of homes, small towns, or sections of larger towns. The Laboratory, working with NEDO and the county, will be researching how to make that option work on both a technical level and a business level.”

The project will be set up as a research and demonstration project. Jonietz continues, “We will use the Lab’s strength in modeling and simulation to come up with a decision-support program and a generic control system that could serve as a blueprint for incorporating renewables and smart grid technology into the nearly 1700 public and cooperatively owned utilities across the United States.” That market buys close to 25 percent of the nation’s electric power.

The main capital investments for the Los Alamos-NEDO project (see figure below) are two 1-megawatt (MW) solar PV arrays connected to two commercial-size batteries, which are controlled by a micro energy management system (micro EMS). The system will be constructed on a capped landfill near the Laboratory, and its power output will be fed directly into the low-voltage side of the nearby substation, where power coming in on high-voltage transmission lines is transformed to a lower distribution-level voltage. The power will then be distributed to the town through the county utility’s distribution feeder lines and to the Laboratory through the Lab’s distribution system.





Left to right: Andy Erickson, Rafael de la Torre (electrical engineer for the county utility), Dr. Satoshi Morozumi, Karl Jonietz, and John Arrowsmith in downtown Los Alamos after finalizing agreements with Japanese industry representatives.

The Los Alamos County Department of Public Utilities, led by John Arrowsmith, will construct one of the 1-MW solar arrays. Erickson, who as Laboratory representative purchases 80 percent of the power coming into the county, will back that investment by guaranteeing to purchase power from the array. The arrangement will support the smart grid project and will help the Laboratory meet the federal requirement that by 2012 all federal sites purchase 7.5 percent of their power from renewable sources.

The rest of the installation (solar array, batteries, and micro EMS) will be a demonstration of NEDO-contributed solar and smart grid technology. NEDO fosters greater use of new energy and conservation of energy by promoting research and development collaborations among Japanese industry, universities, and government. NEDO leaders chose Los Alamos to host this utility-scale demonstration because of the county utility's willingness and ability to institute rate incentives without permission from the state regulatory commission. NEDO is also interested in working with the Laboratory on technology standardization and other issues related to the smart grid. In addition, the Japanese see this project as opening doors to a future U.S. market dependent on renewables.

NEDO's Dr. Satoshi Morozumi remarks, "This type of utility-scale system will help get PV systems into the U.S. grid and will get community utilities into a good position relative to the wholesale market. By having their own PV resources, they can choose when to buy power and when to generate their own."

This sounds good, but it works only if the solar fluctuations on the local array can be balanced. The monthly bill for each local utility has two parts: an energy charge for the total number of kilowatt-hours used and a demand charge for the highest average rate of energy use (number of watts) recorded during any 15-minute period. (The demand charge pays for the excess generating capacity and transmission capacity needed to meet peak demand.) If you're unlucky and the local solar output dips just when consumer demand peaks, the local grid will draw power from the main grid at just the wrong time, and the monthly demand charge will go way up, defeating efforts to reduce costs.

To help avoid those situations, Erickson, wearing his utility hat, is making the Laboratory's infrastructure available as part of the smart grid project. Three on-site generation sources (a diesel generator, a gas turbine generator, and a steam turbine) might be used. Also certain large electrical loads (a wastewater pump at the Laboratory's water treatment plant and the air-conditioning system for the Lab's seven-story NSSB administration building) will be outfitted with smart meters and converted into demand-response loads that will be used to balance fluctuations in solar output and smooth out demand through the day. In addition, Erickson and Arrowsmith are working to bring online a new hydroelectric resource, a low-flow 3-MW turbine at Abiquiu dam, which could be used to smooth fluctuations from the solar array. The county's potable water pumps and storage tanks are also potential demand-response loads.

Misha Chertkov, leader of a separate Laboratory Directed Research and Development (LDRD) theoretical project on smart grid stability comments, "In principle, the county and the Lab can be very creative about controlling these variable sources and commercial-size loads. They could smooth out the fluctuating output from the solar arrays so well that PNM [the utility that controls much of the regional grid in New Mexico] wouldn't be able to detect that the county had put a solar

Left to right: The Lab's Andy Erickson, Scott Backhaus, and Loren Toole are honing plans for the Lab's end of the smart grid project.

array on the grid. If we can develop and demonstrate such automated control schemes, the solar integration problem will be solved, and other municipalities can copy what's being done in Los Alamos."

The control schemes will be designed from statistical descriptions of the frequency and duration of fluctuations in sunlight and from analyses of the response times and flexibility of the variable sources and demand-response loads being contributed by the Lab and the county. Scott Backhaus, a Laboratory experimental physicist and the second principal investigator on the Los Alamos-NEDO smart grid project, is being supported right now by the DOE's Office of Electricity to perform those analyses and develop control schemes. Backhaus won't be alone. Chertkov, Russell Bent, and other project theoreticians in the LDRD smart grid project are developing general mathematical approaches that likely will prove very helpful.

Control schemes are rules for deciding which power sources or demand-response loads to bring into play to balance supply and demand, given the county's price signals, weather, charge on the batteries, and so on. The rules, rather than being used independently, become one component of a the utility control system: the "brain" in a smart grid.

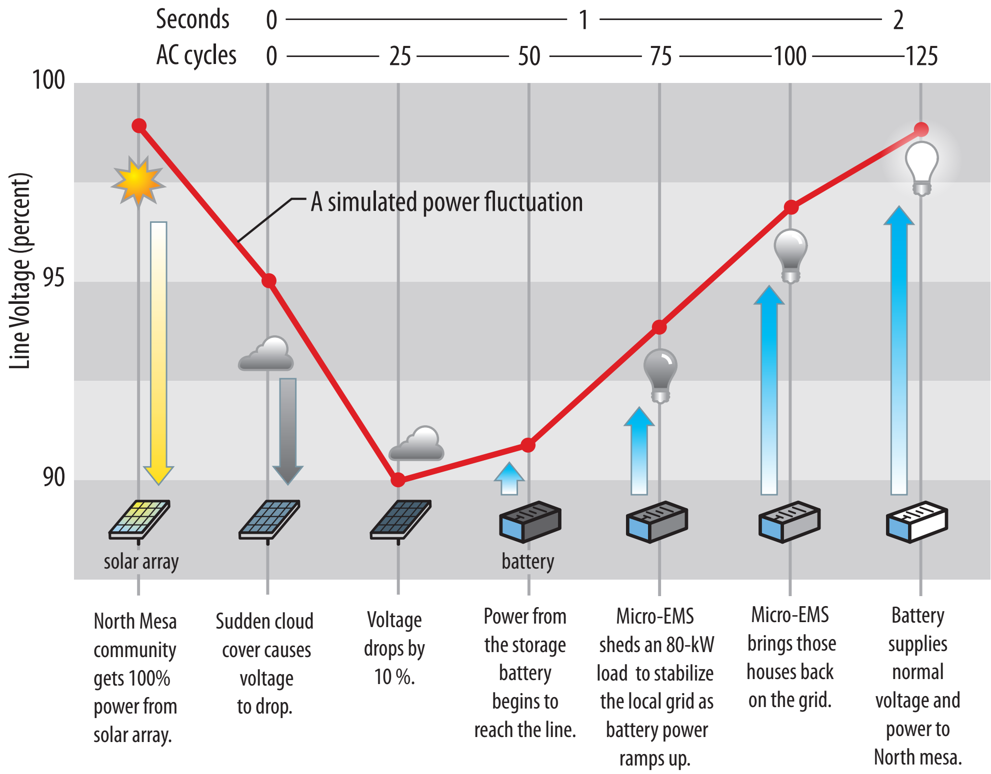
A second component of the control system is being developed by Toole and his colleagues from an advanced grid simulator called TRANS-EX, created in 2009 to determine the transmission elements that would be needed to gather 20 percent of the grid's total power from wind farms. Whereas Backhaus's control schemes will forecast the power available to meet demand, Toole's simulator will recommend distribution-level actions to operators.

Testing High-Penetration Solar

Even before NEDO chose to site its demonstrations in Los Alamos, Toole used TRANS-EX to create a live computer simulation of a scenario of great interest to NEDO—namely, how the North Mesa neighborhood grid in Los Alamos would respond if the proposed NEDO solar array and battery system were the sole supplier of power (called 100 percent penetration) and suddenly clouds covered the solar array.

The simulation (above) showed how the micro EMS could shift the North Mesa load from the solar array to the battery during a sudden cloud cover. Switching from solar to battery power took just over 2 seconds but involved shedding load by disconnecting about 30 houses for 0.3 second, demonstrating a downside to 100 percent penetration.

This example illustrates the type of information that will come through simulation and live experiments on the Los Alamos-NEDO project. That information can then make its way into a cost-effective control system for balancing solar power fluctuations on a locally run grid.



More Power to the People

Chertkov explains the importance of local control, "In computer science we've learned that it's efficient for different processors to solve different scales of the same problem. Similarly, smart grid control needs to be distributed over many scales. If counties like Los Alamos are nodes in a huge grid, and each node balances its own power fluctuations, then whatever fluctuations remain could be taken care of at a larger scale. But without the smaller-scale control, fluctuations can grow and lead to rolling blackouts. If we solve the control problems, distributed power generation brings so many benefits—a healthier environment, a more-stable grid, more local control, more self-sufficiency, and less risk of rolling blackouts."

"Many locations have the potential to incorporate renewable energy into their mix of power sources," adds Jonietz, "but they lack the tools to do so cost-effectively. If the Los Alamos-NEDO project is successful, the Lab hopes it will result in decision-support software that could be licensed commercially and used daily by small utilities in the West and overseas." ❖ LDRD

—Necia Grant Cooper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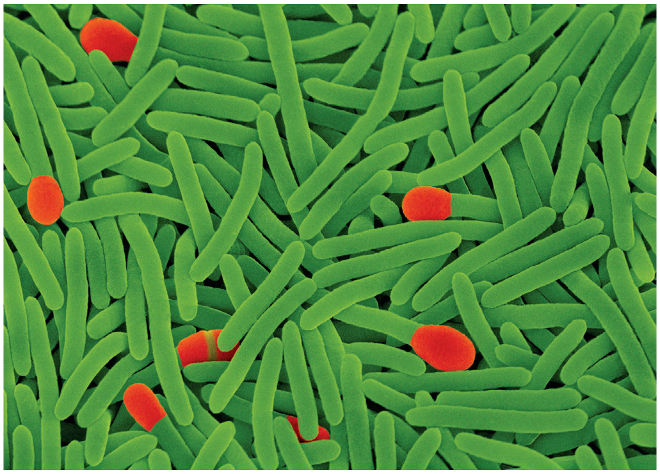
Metagenomics

A novel technique for surveying the genetic makeup of the complex soil ecosystem is paving the way for a wide range of new applications, including better greenhouse gas management.

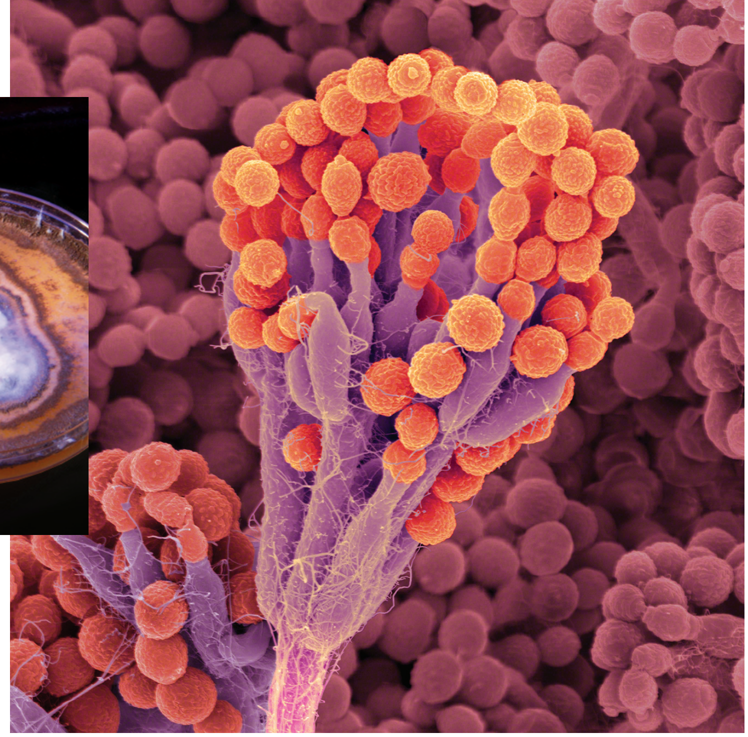
There is an invisible world all around us. Air molecules mix and mingle. Radio waves course silently by. And in the soil under our feet, countless trillions of microscopic organisms perform important ecosystem services. They break down plant matter, protect crops from disease, and filter the groundwater. Yet less than 1 percent of them have been studied in a laboratory. Most of their activities—and most of the organisms themselves—remain unnamed and unexplored by science.

Our ignorance of this "secret life of dirt" is no small omission. For example, as carbon dioxide (CO_2) levels rise in the atmosphere, plants absorb this greenhouse gas during photosynthesis and use its atoms to construct broader leaves, taller stalks, and bigger roots. When plants shed their leaves, recycle their roots (which happens yearly), or die, the microorganisms (microbes) in the soil go to work on them, resynthesizing and freeing some of the CO_2 the plants previously absorbed. How much CO_2 is returned to the atmosphere by these microbes, and how much remains in plant matter in the soil? Embarrassingly, no one knows. No one knows for certain what role the soil itself plays in the atmospheric changes that cause global warming. But Los Alamos scientist Cheryl Kuske, together with her colleague John Dunbar and a talented lineup of postdoctoral researchers, technicians, and students, is changing all that with a sweeping approach to genetic study called *metagenomics*.



Clostridium bacteria like these are abundant in soils, and many species are known to degrade plant matter, which affects how much carbon is stored in the soil and how much is returned to the atmosphere as CO_2. CREDIT: DENNIS KUNKEL MICROSCOPY INC.

Traditional microbiology lab work entails studying the genetic information from a single organism grown in a culture. Metagenomics, on the other hand, works directly with the complex mixture of DNA found in samples taken from the natural environment—in a soil sample, image for instance. While a genome is the complete set of genetic information for a particular organism (for example, the human genome), a metagenome is the complete set of genetic information for an entire community of organisms, and metagenomics describes the gathering and processing of this rich swath of biological information. It is within such community-level biological



Denizens of the dirt: Petri dishes (above) harbor various fungi that Kuske isolates in order to study new species involved in degrading plant matter. Their genetic information is added to a database that Kuske compares against gene sequences found in various soils. *Penicillium* (right) is an example of a fungus that's commonly found in soils (and is the originator of the antibiotic penicillin). CREDIT: DENNIS KUNKEL MICROSCOPY INC.

information that Kuske finds answers about CO_2 processing and other soil-related environmental issues.

A soil metagenome is a diverse and complicated thing. On average, one gram of soil contains at least a billion microorganisms. Those billion organisms typically span thousands or tens of thousands of different species (Dunbar and other colleagues have shown that this number can even range up to millions of different species), representing all three major biological domains of life. Worldwide, microbes from two of these domains, archaea and bacteria, contain about as much carbon in their cells as the entire plant kingdom, and about ten times more nitrogen- and phosphorus-based nutrients. The third domain, eukarya, is made up of plants, animals, and others, including fungi—microbes that are essential for plant survival and supply key products for human use, such as antibiotics and yeast. In other words, the underground microbial world, while largely unknown, is far from unimportant. And metagenomics is only just beginning to bring the vast majority of these microbes and their activities within range of discovery—and perhaps appropriation for human benefit.

"Although these organisms are microscopic, they collectively impact human activities and the Earth's processes at regional and global scales," Kuske says. "And most of their roles are beneficial." Indeed, the lure of such beneficial, collective impacts is part of what makes soil metagenomics so promising. Emerging technologies derived from microbes hold the potential for revolutionary advances in human health, industry, biofuel, greenhouse gas absorption, and even the cleanup of large-scale environmental contamination. With all this on the line, scouring every microbe's every gene by traditional methods might seem inadequate. "We have all these really pressing environmental issues, and we don't have time to do this step by step," Kuske asserts. "We have to jump."

Fragmented Approach

In Kuske's research, soil samples are collected and brought to Los Alamos from a variety of carefully controlled study sites around the country (see "Open-Air Laboratories," facing page). Her team extracts DNA from all the cells in a small vial of soil by bursting the cell walls and membranes and capturing the DNA as it slithers out. Then an advanced, high-throughput DNA sequencing apparatus "reads" the DNA and outputs the genetic sequence as an ordered list of four letters, like "ACCGTGTCAG," in which A, C, G, and T represent bases (as opposed to acids) found in DNA. Since DNA is double-stranded, and each base is naturally paired with a complementary base, scientists refer to this small unit of genetic information as a "base pair."

In general, living cells function by using the sequences of bases in their DNA as a blueprint for assembling proteins. A particularly important type of protein is the enzyme, because only when the right combination of enzymes is present and active do cells carry out various functions, like metabolism or replication. So DNA specifies particular enzymes, and the enzymes enable particular functions; the DNA sequence that encodes for one enzyme is called a gene.

But even with state-of-the-art sequencing technology, there are experimental limitations to how much genetic information you can gather about the microorganisms found in a complex mixture like soil. You don't get entire

Open-Air Laboratories

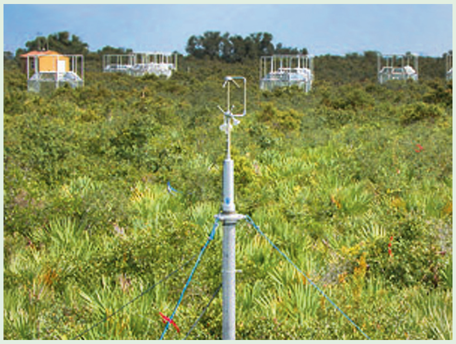
For over a decade, the U.S. Department of Energy has managed a collection of large, outdoor field experiments to monitor the effects of elevated CO_2 levels in real ecosystems. Observing stations and CO_2 injectors were established in a variety of ecological zones, and researchers have been collecting empirical data on how the extra greenhouse gas in the air affects the plants and other life present.

Kuske's team takes its soil samples from six of these study sites, chosen to span a diverse range of habitats within the United States. In most of the sites, plant growth increases in response to the elevated CO_2. But how much of that carbon remains locked up in plant matter, safely out of the atmosphere? That depends on the microbes in the soil, and it is one of Kuske's principal research objectives to assess the microbes' response to the added CO_2, an effort that began in earnest about a year ago. One of the major challenges is to identify trends in microbial populations that are important at the landscape level, which requires many samples and a blend of metagenomic and other measurements.

Kuske's early results show that a soil community's response to the enriched CO_2 atmosphere is varied and complex; each ecosystem has a different response pattern. At some sites, the total microbial biomass goes up or down. In some cases, the fungal populations appear to change the most, while in others it's the bacteria. In the Nevada desert site, for instance, there was no observed change in fungal populations, but a population of bacteria called cyanobacteria diminished substantially. This may be significant because cyanobacteria in arid lands are responsible for many of the services normally provided by plants elsewhere: absorbing carbon from the air through photosynthesis, fertilizing, and stabilizing the soil against erosion. Arid lands—including deserts, arid grasslands, and shrub lands—make up one-third of all the land on Earth.

Sweetgum plantation in Tennessee
PHOTO COURTESY OF STEVE EBERHARDT / ORNL

Desert shrubs, grasses, and soil crust in Nevada
PHOTO COURTESY OF LYNN FENSTERMAKER

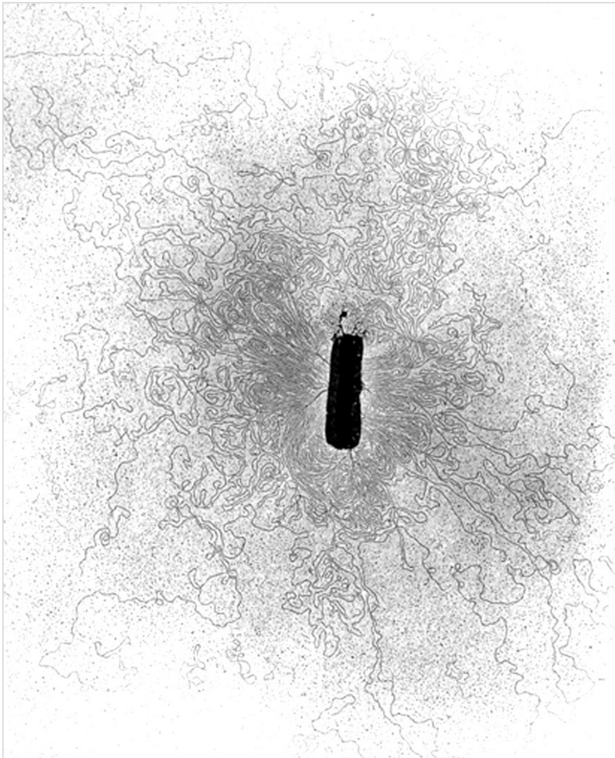


Palmetto and scrub oak grove in Florida
PHOTO COURTESY OF BERT DRAKE

Estuary marsh grasses in Maryland
PHOTO COURTESY OF MARK SIGRIST

Pine forest in North Carolina
PHOTO COURTESY OF YAVOR PARASHKEVOV

Aspen, maple, birch, and poplar plantation in Wisconsin PHOTO COURTESY OF DAVID F. KARNOSKY



An electron microscope reveals DNA emerging from a bacterium whose membrane has been ruptured.
CREDIT: SCHOOL OF BIOLOGICAL SCIENCES, UNIVERSITY OF TEXAS, AUSTIN

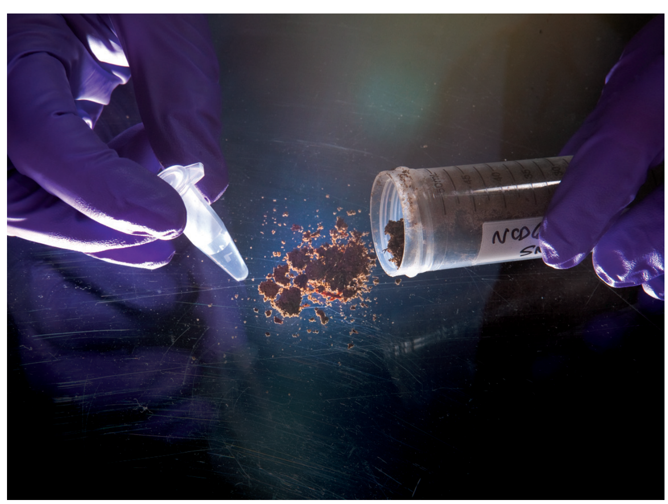
genomes for each microbe in the sample. You get DNA fragments because the DNA itself is brittle and because the sequencing machines can't read sequences beyond a few hundred base pairs—fewer than the thousand or so base pairs in an average bacterial gene. In a typical soil experiment, the sequencing machine might output hundreds of thousands of these different fragments, but there is no obvious way to know which fragments do what for which microbe, since the overwhelming majority of the DNA sequences found in soil communities are not yet known to science. (And a small fraction of the soil DNA isn't microbial at all, but rather comes from bits of old plant matter, dead insects, and so on.)

The situation is akin to waking up in a large library building in a foreign country and being asked to describe the content of everything in the entire library. There's too much information, and you don't know the language very well. In fact, the metagenomics problem is thornier than that: Since researchers have only tiny DNA fragments to work from, it's more like a library with only a few random pages from each book! Still, you might recognize a few words or concepts that come up often (analogous to recognizing base pair sequences for known genes), and you might recognize a page from a certain type of book, like a dictionary or a travel guide (analogous to recognizing a sequence from a known organism). Now what you need is some kind of procedure for understanding every book in the library—what to look for, which paragraphs to scan, when to move on, and so forth.

There are essentially two approaches to pursue. You could take a targeted approach, searching every page for occurrences of the words or concepts you already know. This might give you a sense of the prevalence of that concept in this foreign culture or allow you to track variations on its theme. Similarly, scientists can focus on a known type of gene—one that helps fungi digest dead plant matter, perhaps—and learn about its prevalence or variety within the soil community. This is called "targeted metagenomics." In the other approach, you could just skim everything in the library, looking for familiar patterns in the language. When biologists take this approach, directly sequencing whatever DNA is present in the hope of finding familiar sequences (embedded in unfamiliar genes) that might lead them to new enzymes or new species, it's called "shotgun metagenomics." Kuske's team uses both targeted and shotgun approaches.

Targeting Consequences for Humanity

For targeted metagenomics, Kuske uses a common laboratory technique known as polymerase chain reaction (PCR) to search for genes in the DNA extracted from soil. The process involves using certain known sequences called "primers" that are designed to locate and attach to a particular sequence within the soil DNA. These primers might seek out the common beginning and ending sequences for a particular class of genes whose variations, from one species to another, occur only between these endpoints. In fact, it is frequently necessary to choose primers to bracket only a small part of one gene, since sequencing reads are limited to less than a few hundred base pairs. The PCR process selectively retrieves the bracketed DNA from the sample and makes copies to be sequenced. That's the targeting: only the chosen gene fragments are sequenced,



DNA is stored in a small vial of clear liquid after being extracted from a soil sample.

not the complete jumble of everything present in the soil.

Kuske's group is developing primers for many genes that can be used to identify organisms or their functions (enzymes). She has been "fishing," as she calls it, for certain specific genes so far, with many more to come. One gene she targets, for example, is called the rRNA gene and is present in all living cells. Every species known has a unique version of this gene, which allows biologists to use it to classify all life forms. So when researchers target this gene, they can track the populations of various microbes in selected environments—in normal versus elevated-CO_2 environments, for example—based on the number of occurrences of each version of the gene they find. This works for all organisms, whether or not they have been studied in a laboratory before; even unnamed life forms can be tracked through their unique rRNA genes. The result is a complete picture of population numbers, population shifts, and population diversity in the soil sampled.

Los Alamos scientists Cheryl Kuske and John Dunbar prepare multiple soil DNA samples (dyed blue) for sequencing.

Another gene they track is responsible for making cellobiohydrolase, an enzyme that some fungi use to break down cellulose, the main component in plant matter. In a CO_2-enriched environment, there is more plant growth because plants convert some of the extra CO_2 into extra cellulose. This might sound reassuringly self-correcting: more CO_2 (bad) yields more plant growth to absorb more CO_2 (good). But if the extra plant matter is ultimately digested with cellobiohydrolase, then the extra absorbed CO_2 just gets released and returned to the atmosphere. So it's all about knowing how much CO_2 is being recycled, which is partly dependent on how much cellobiohydrolase is in play. Kuske's team is working on that, and models of how the Earth responds to climate change will eventually need to account for this type of soil activity.

Targeting fungal cellobiohydrolase is a powerful way to follow CO_2 recycling from cellulose in the soil. But how can scientists find out if there are other microbes that might perform a similar function, perhaps with a different enzyme? The answer lies in a technique called stable isotope probing.

Isotopes of the same element differ only in the number of neutrons in each atom, so they have different masses but behave identically otherwise. At Los Alamos, the research team enriches cellulose with carbon-13 (instead of the much more common carbon-12) and adds this artificially heavy cellulose to the soil sample.

"This technique essentially follows the adage, 'you are what you eat,'" explains Stephanie Eichorst, a postdoctoral research scientist on Kuske's team. Once the microbe digests the heavy cellulose, its "body," including its DNA, becomes enriched in carbon-13. Now, metagenomic DNA can be separated in a centrifuge, which forces the DNA that's enriched with the heavier carbon to sink. If researchers use only the enriched DNA, then whatever genes they target and sequence must belong to the organisms that are actively consuming the cellulose. Stable isotope probing, therefore, can be used to identify which organisms are performing a particular function (digesting cellulose in this case) since it's always possible to target a gene that's unique to each particular microbe. By this approach, Kuske and Eichorst discovered (heavy) genes from a variety of bacteria and fungi that were not previously known to be involved in degrading cellulose. Further study and genome sequencing of these individual organisms should identify new ways in which they digest cellulose (with new enzymes) and new genes to target in future experiments (corresponding to those new enzymes).

Much can be accomplished with targeted metagenomics. Targeting the rRNA gene gives you population statistics. Targeting cellobiohydrolase gives you data on plant degradation and CO_2 release. And adding stable isotope probing gives you the specific organisms responsible, possibly providing valuable leads about which enzymes and which genes to study next. But what if you don't filter out part of the DNA by targeting only particular genes? What's possible when you sequence all the DNA you find in an ecosystem, using the shotgun approach, and then analyze those sequence data with a computer?

Shotgun Wedding

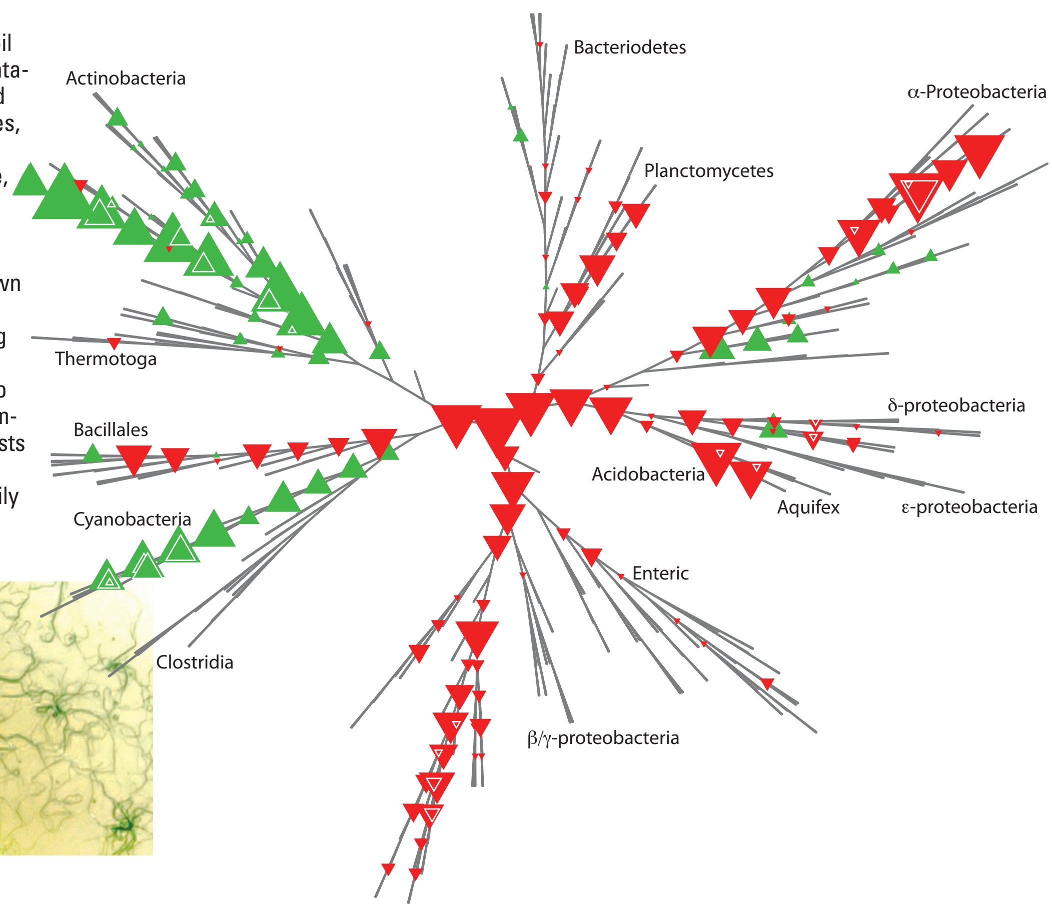
The marriage of biology and sophisticated computer data processing offers tremendous opportunity for advancing bioscience. What's at stake is a deeper, richer understanding of the tree of life, including knowledge of new genes and new organisms and how they co-evolved, as well as several important new applications.

While targeted metagenomics is a story of demonstrated new capability, shotgun metagenomics is still largely a story of potential. To realize that potential, researchers must learn to recognize segments of new genes when they're buried in an avalanche of unknown sequences. But as the collection of known genes grows, the shotgun approach becomes more powerful.

In principle, progress can be made by bootstrapping: Start by identifying a particular gene fragment of interest from a shotgun sample. This gene fragment could be chosen because it contains a sequence that's familiar from another organism; perhaps it encodes for a feature found in some known proteins. Study that gene and perhaps the entire genome it belongs to by traditional methods, and then use the results to expand the database of known sequences.

In practice, however, just identifying a gene fragment to study in a shotgun dataset can be a challenge. With only a few hundred thousand sequence fragments obtained from a billion microbes, and each fragment much shorter than a complete gene, you usually don't get enough genetic data to recognize even a single gene. So Kuske teamed up with computational, theoretical, and genome sequencing colleagues at Los Alamos to pioneer methods of computer-based analysis of very short, recurring base pair sequences that match pieces of known genes. In other words, if you can't recognize enough of any sequence to connect it with a particular gene, then set your sights a little lower: aim to recognize much shorter sequences, up to about 30 base pairs, that have been found before in multiple genes. It is often the case that different organisms share such blips of genetic material because the biochemical function they encode for is common to a variety of living cells. Sometimes it just takes a little handhold like this to obtain clues about which genes or which organisms to study in more detail. If the mini-sequence is somehow connected to photosynthesis, for example, then it could be related to some variety of cyanobacteria, which perform photosynthesis.

Important results are already emerging. Nick Hengartner, from the Los Alamos Information Sciences group, is the team lead for a Lab-directed R&D project to perform the computational analysis of the shotgun data. He and Kuske have been successful at identifying very short gene fragments from shotgun samples and sorting them into different branches of the bacterial "family tree" (see figure below). Doing this provides a quick snapshot of the distinctive features of the bacterial population in a particular environment. Shotgun data also allow biologists to add to the family tree whenever they find new base pair sequences that have sufficient overlap with known bacterial sequences to allow them to pinpoint the right branch of the tree. With more time and effort, researchers expect to identify unknown



Soil census: Shotgun data from two distant soil collection sites are compared in this representation of the bacterial family tree. The green and red triangles indicate increases and decreases, respectively, in the population of different bacteria found in a Nevada desert soil sample, relative to soil from a Tennessee sweetgum plantation. The strip of green triangles at the eight o'clock position, for example, shows the increased role of various cyanobacteria (shown in the photograph); these bacteria make up for the lack of desert vegetation by performing many of the functions normally performed by plants, including photosynthesis. In addition to displaying population trends, this diagram demonstrates the capability of Los Alamos scientists to associate short sequences obtained from shotgun methodology with locations on a family tree—an essential ability for identifying and placing new species as they are discovered.

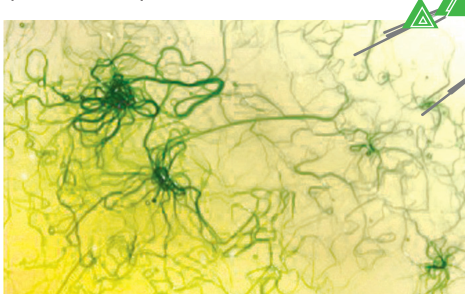


PHOTO COURTESY OF CHERYL KUSKE

Metagenomics to the Rescue

Researchers envision a variety of practical applications to come from metagenomics in the future, with many of these applications addressing critical human needs. In each of the following examples, rapid metagenomic studies of the relevant microbial community could allow us to duplicate, harness, or expand upon the special capabilities of microbes.

Medicine: Many drugs in widespread use today, such as antibiotics, derive from microbes or plants, but most of this natural biodiversity remains untapped. Metagenomic exploration of the remaining biodiversity could lead to the rapid discovery of new medicines. Additionally, the community of bacteria living in and on the human body, especially in the intestine, plays a major role in the regulation of human health. Using metagenomics to examine this community could vastly improve our understanding of nutrition and disease.

Climate: A bacterial group called cyanobacteria, largely in the oceans, performs about half of all photosynthesis on Earth. That, together with carbon cycling by soil microorganisms, exerts a substantial influence on the atmosphere and therefore the climate. Metagenomics is already helping us begin to understand the role of microbes in climate change and may help us identify species and enzymes capable of slowing or reversing that change.

Bioenergy: Cellulosic ethanol, a renewable fuel resource, is manufactured from plant cellulose found in agricultural waste, such as corn stalks, wheat straw, and switchgrass. Microbes working together are used to first turn cellulose into sugars and then ferment those sugars into cellulosic ethanol fuel. Metagenomics can provide the additional information we need to learn how to adapt microbial fuel production to widespread application.

Agriculture: Soil microbes are known to protect plants from disease and to provide them with nutrients, as when they convert atmospheric nitrogen gas into useable ammonia. Such abilities might someday be manipulated for improved crop output, but first we need metagenomic analysis to improve our understanding of these complex community activities.

Environment: Much natural and human-made waste is beneficially processed by microbes. Gasoline, for example, leaks from the fuel tanks under many gas stations and enters our groundwater. But our drinking water is made safe by microorganisms, and the same capability could be exploited to clean up larger-scale environmental damage, such as oil spills. Metagenomics could allow us to identify the microbes and the waste treatment processes needed to handle the ever-expanding collection of chemicals that we introduce into the natural environment.

organisms, determine their roles in the ecosystem, and even predict their responses in the face of changing environmental conditions.

Shotgun metagenomics also offers the potential for valuable new applications. In theory, it should someday be possible to search any well-studied metagenome—in soil, ocean water, caves, digestive systems of animals, and so on—for a specific enzyme of interest. With all the diversity we observe in Earth's microbial communities, it is likely that nature has already evolved biochemical solutions to meet many of our needs. Moreover, the human body is itself a major bacterial community, and comparing bacterial metagenomes across different human populations might allow researchers to quickly identify medically significant features. For example, a shift in the relative abundance of two different types of bacteria in the human gut appears to be at least partly responsible for causing obesity. (See "Metagenomics to the Rescue," above.)

Today, of course, the results remain more modest. Kuske and her team have uncovered trends in microbial populations in different habitats, with and without increased CO_2 levels. They have identified organisms that break down cellulose and release CO_2—organisms that had been previously unknown to do so. They found that a version of the gene for cellobiohydrolase, employed to break down cellulose, is present in most known fungi. And they are collecting data on how much CO_2 the major soil communities can be expected to re-release into the air as global warming continues. Metagenomic research is a bold new initiative, and these early results—those pertaining to our immediate environmental needs—are just the beginning. ❖ LDRD

—Craig Tyler

SPOTLIGHT

Clean Air and Abundant Fuel

To reduce carbon emissions from the exhaust stacks of coal- and gas-fired power plants, we might enlist the help of an enzyme found within our blood. The enzyme, called carbonic anhydrase, combines carbon dioxide with water to form bicarbonate ions and protons. If it were used to perform that same chemistry in a power plant's exhaust stream, the resulting bicarbonate could be converted into calcium carbonate, a solid that could be safely stored away or used in making everyday materials like plastic or cement.

The same carbon conversion reaction could also make carbonic anhydrase valuable for growing algae capable of making oil for fuel. The algae-to-fuel conversion process has already been solved, but growing the algae is prohibitively time consuming. However, these algae take up bicarbonate directly, which means that if we could add carbonic anhydrase to algae ponds, the enzyme would rapidly convert carbon dioxide from the atmosphere into bicarbonate—feeding the algae and greatly accelerating their growth.

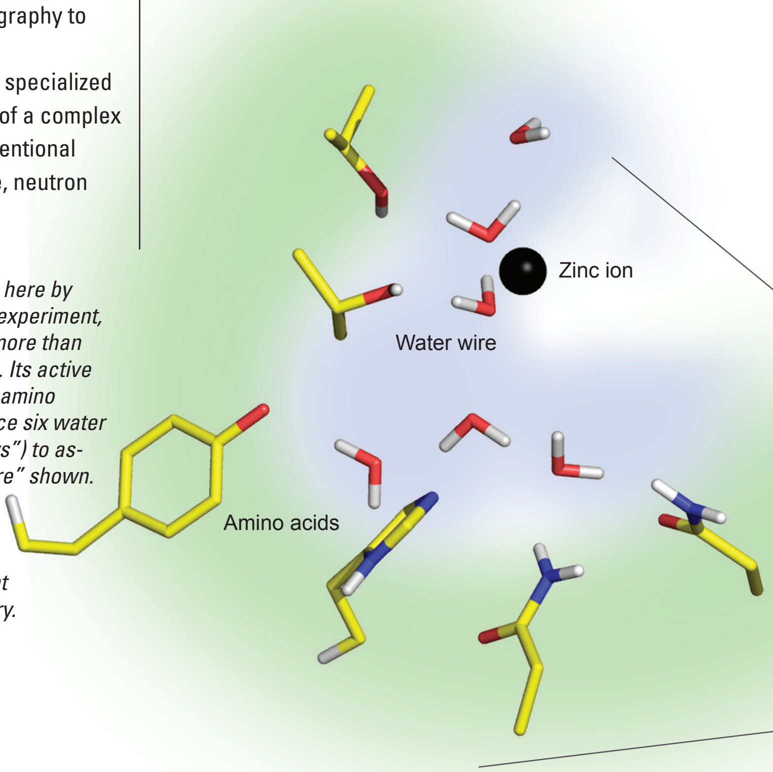
Los Alamos bioenergy scientist Zoë Fisher is working to design a high-performance version of the enzyme for both settings: exhaust stacks and algae ponds.

To do that, she needs a clear picture of the molecule she's working with. Carbonic anhydrase is a single molecule made up of more than 3000 atoms, but the conversion from carbon dioxide to bicarbonate takes place within just a small pocket of the structure known as the "active site." Inside the pocket, a zinc atom is bound to hydroxide, making $ZnOH^-$. If a carbon dioxide molecule (CO_2) ventures too close to the pocket, the hydroxide "attacks" it to form $ZnHCO_3^-$, zinc bound to a bicarbonate ion. Then a water molecule from the surrounding fluid displaces the bicarbonate ion (HCO_3^-), leaving ZnH_2O in the active site and setting the bicarbonate ion adrift, to be stored as calcium carbonate or fed to algae.

But in order to convert another CO_2 molecule, the active site must be reset. That is, the ZnH_2O must be changed back to $ZnOH^-$ through the loss of a proton (H^+). The speed of the reset step is known to limit the rate at which the entire enzymatic reaction can occur, but many details about this step—especially how the proton is transferred away—have only recently come to light, thanks largely to Fisher's successful application of neutron crystallography to visualize the active site.

Neutron crystallography is a specialized technique for making an image of a complex molecule. Unlike the more conventional x-ray crystallography technique, neutron crystallography allows you to see hydrogen, the smallest atom. The exact location of the hydrogen atoms turns out to be critical because in carbonic anhydrase, they appear in a row of six water molecules (H_2O) that are held in a precise arrangement by the amino acids found in the enzyme's active site. It is this "water wire" that is responsible for resetting the enzyme by channeling the unwanted proton down the "wire" and away from the active site. Because water molecules are polar—positively charged at one end and negatively charged at the other end—their exact orientation determines the arrangement of electrical forces that steer the positively charged proton away.

Fisher and collaborators at the University of Florida were able to use the Protein Crystallography Station at the Los Alamos Neutron Science Center—currently the only instrument capable of revealing the exact positions of hydrogen atoms in enzymes—to see the structure of the active site, including the water wire (see figure below). With this information in hand, Fisher can redesign carbonic anhydrase by swapping out amino acids in the active site, thus changing the orientation of the water molecules in the water wire. The resulting alteration in



Carbonic anhydrase, as revealed here by Fisher's neutron crystallography experiment, is a single molecule made up of more than 3000 atoms (green "ball" at right). Its active site (exploded view) contains six amino acids (yellow molecules) that force six water molecules (red and white "elbows") to assume the shape of the "water wire" shown. Improving the way the water wire generates electrical forces to push protons out of the active site could lead to important applications in the energy industry.

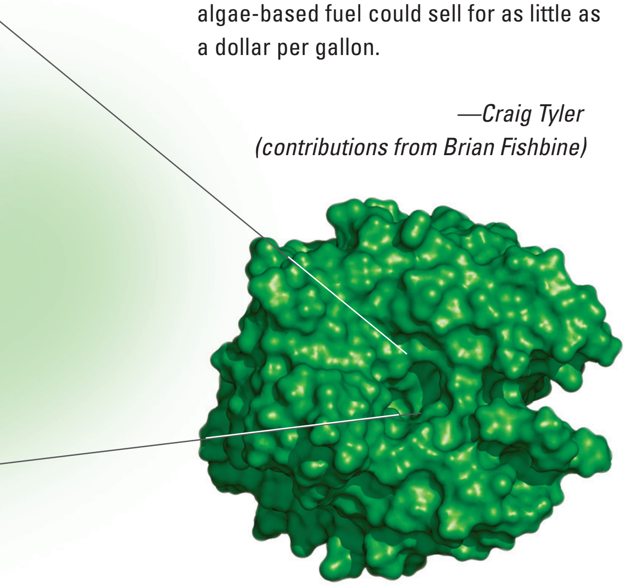
electrical forces should make for a more effective proton transport channel.

The enzyme will also need to be tailored to each specific application. To function in a power plant's exhaust stack, the enzyme must be able to withstand high temperatures. This stability can be achieved by redesigning the structural "scaffold" of the enzyme (the green "ball" on the right in the figure), rather than the functional active site. Fisher's colleague Csaba Kiss from Advanced Measurement Science has developed a unique approach to do just that. It could take two or three years, but Fisher and Kiss are extremely confident that it will work.

To serve as a growth accelerant for algae, the enzyme will have to operate at a higher pH range (acid-base scale) than it experiences in its natural environment—human blood—which is always very close to pH 7.4 (neutral is pH 7). Algae, on the other hand, tend to push the surrounding water to pH 9 or above, where carbonic anhydrase does not work very well. (Nor should it have to: as Fisher points out, "If your blood were this basic, you'd be dead for sure.") To overcome this limitation, she'll need to select different amino acids for the active site, to make the water wire better suited to the higher pH.

If these efforts are successful, and if reasonable economies of scale are achieved, we could see substantial advances in clean electricity and home-grown fuel production in just a few years. And while you might expect that this kind of near-term energy security doesn't come cheap, consider this: the new algae-based fuel could sell for as little as a dollar per gallon.

—Craig Tyler
(contributions from Brian Fishbine)



Shooting Rocks on Mars

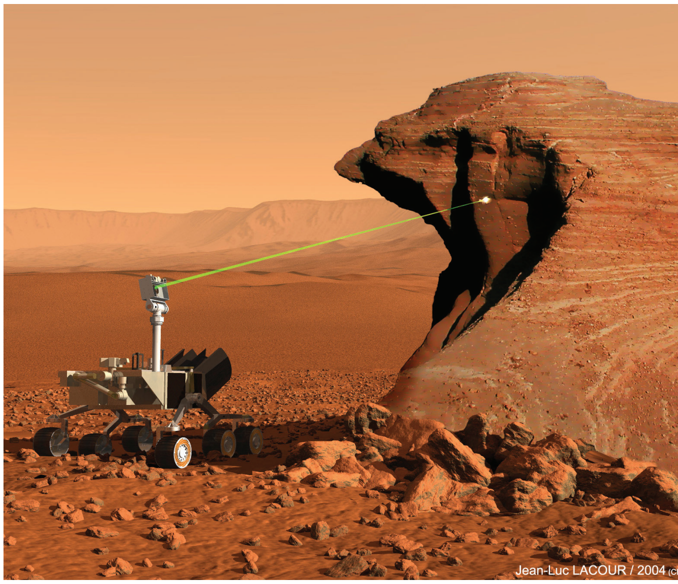
Science fiction laser weapons blast enemy aliens, but ChemCam, an instrument Los Alamos developed in collaboration with NASA and the French Space Agency, will aim its laser at Mars rocks.

Delivered in August 2010 to NASA's Jet Propulsion Laboratory in California, ChemCam is being installed on the Mars Science Laboratory, a six-wheeled rover named Curiosity that will be launched on a rocket in 2011 and lowered by cable to the Mars surface from a hovering drop ship in 2012. NASA is arming the rover with numerous scientific instruments in hopes of learning if the planet was ever able to support life. Curiosity will examine the Mars environment for two Earth years (one Mars year).

ChemCam comprises two of the rover's instruments: (1) a remote micro-imager for taking high-resolution pictures and (2) laser-induced breakdown spectroscopy (LIBS) equipment for chemically analyzing rocks and soil. The Laboratory's Roger Wiens, whose Space Science and Applications team miniaturized the LIBS technology for space, will lead a team of U.S. and French scientists operating ChemCam and checking the LIBS results from Mars.

LIBS works remotely. From a mast atop the rover (see illustration), its high-energy pulsed laser can hit targets up to 7 meters (about 23 feet) away, dislodging atoms at very high energy—"They're just zinging off of there," says Wiens—and exciting them to an electrically charged state: a plasma dot that gives off light as it loses energy. A telescope (also on the mast) collects the light and focuses it onto the end of a fiber-optic cable linked to the LIBS spectrometers in Curiosity's body. The spectrometers resolve the light into wavelengths that reveal the specific types and amounts of elements in the rock. Pre-analysis laser pulses can even remove dust and weathered coatings to prepare the rock for analysis.

"And LIBS recognizes almost all known elements," says Wiens. It's this elemental information that will characterize the planet's makeup and pinpoint samples interesting enough to be physically sampled by other Curiosity instruments.



Curiosity, an SUV-size rover, can remotely analyze otherwise-inaccessible rock and soil samples with its LIBS laser from Los Alamos.

NASA is also considering a proposal to use LIBS to search for water at the Moon's south pole, and Los Alamos's Laboratory Directed Research and Development program is funding experiments that combine LIBS with Raman spectroscopy, a related technology, for possible use on a future Venus lander. LDRD

—Eileen Patterson

Fission Makeup

If there's one thing scientists at Los Alamos National Laboratory know about it's nuclear fission. That's a reaction in which an overly large and heavy nucleus, such as plutonium, absorbs a single neutron and instantly breaks into two different nuclei (fission products) and a few neutrons, releasing nuclear energy. Los Alamos scientists expertly exploited the process, finding ways to unleash large amounts of energy slowly (in a nuclear reactor) or in a flash (in "the bomb").

In the 1940s, Los Alamos scientists developed a method for determining the fission yield—the amount of energy released by fission—of a nuclear device. Individual fission products were isolated from samples of the radioactive debris, and their beta-ray count rates were converted using conversion factors (so-called *K*'s, *Q*'s, and *R*'s) into the number of fissions that occurred in the sample. The number of fissions fed into the fission-yield calculation.

Then 1952 saw the establishment of Lawrence Livermore National Laboratory. Fission gurus themselves, Livermore scientists designed their own bombs and initially, used the Los Alamos beta-counting method to determine fission yields. But Livermore had pioneered a gamma-ray counting method and toward the end of the 1960s, began using it exclusively to determine fission yields. Both methods produced the same results.

That is, until "the problem" showed up.

It began when Los Alamos remeasured some of their conversion factors in the 1970s and found some disagreements with the "historical" values. They determined a new, "modern" set of values and presented their results at a 1977 meeting sponsored by the Department of Energy (DOE), but they didn't exactly use the open literature to call attention to their findings, nor did they use the modern values in their fission-yield calculations.

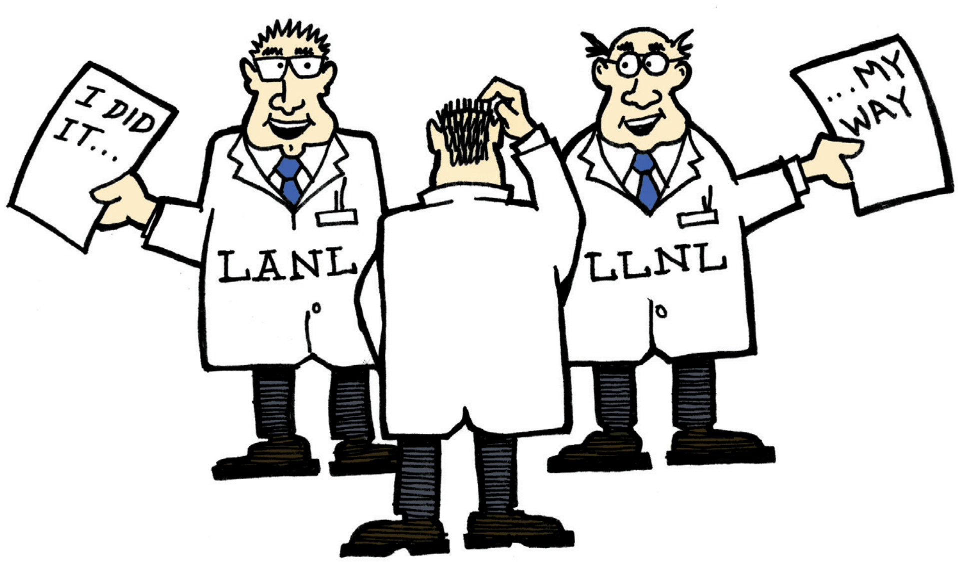
"The differences between the modern and historical values were relatively small," explains Don Barr, former head of the Los Alamos nuclear chemistry group (retired), "and when we calculated new fission yields, they always fell within the error bars of the historical yields. After discussions with some weapons designers, everyone agreed that it was better to maintain consistency and not use the modern values until there was a compelling reason to do so."

That reason began to surface in 1992 with the end of nuclear testing. Assurring the reliability and safety of the nuclear stockpile fell to the Stockpile Stewardship program, which among other things uses a combination of computer modeling, simulation, and non-nuclear tests to develop computer codes that could reproduce 45 years of nuclear test data. By 1995, the codes had become so sophisticated that they needed to be validated against the best data, and that, reasoned the Los Alamos analysts, meant providing the coders with fission yields calculated using the modern conversion factors. So Los Alamos began revising its previously determined yields and suggested that Livermore do the same.

Livermore politely declined, noting that its gamma-counting method didn't rely on *K*'s or *Q*'s or *R*'s; therefore, its fission-yields didn't need revising. And Livermore was mystified as to why, after 40-some years, Los Alamos wanted to fix something that wasn't broken.

The dispute boiled down to fission-product yields (*Y*'s), each of which is the fraction of fissions that lead to the production of a specified nucleus and is not to be confused with the fission-yield. The *K* factors are inversely proportional to the *Y*'s, while the *Q*'s and *R*'s contain ratios of them. Whereas Livermore used the *Y*'s directly in its fission calculations and Los Alamos used the rather clever but funky *K*'s, *Q*'s, and *R*'s, it turns out that Livermore needed to multiply one of its *Y*'s by a Los Alamos *Q* to put both methods on the same fission scale. Capiche?

Don Barr knew all this, but Livermore's post-testing-era analysts did not; that knowledge had not survived a round of retirements. Thus, when Los Alamos argued that at least one historical conversion factor was buried within the computer code that Livermore used to determine yields, Livermore replied it would have to look into it. And, by the way, just where was the documentation on the 1970s experiments,



and would Los Alamos kindly share it?

Sifting through old data is about as appealing as doing one's taxes, and while both laboratories agreed to cooperate, their efforts lost traction, and the problem persisted into the next decade.

But at the urging of DOE and both laboratory directors, the effort to reconcile the differing fission yields gained momentum. Los Alamos, for its part, went through 60 years of in-house reports and laboratory notebooks and conducted an intense evaluation of its conversion factors. Livermore found a historical Los Alamos *Q*-value lurking among thousands of lines of its code and executed a thorough, unbiased review of *Y*'s in the available literature.

In addition, Los Alamos staff from the Chemistry, Theoretical, and X-Computational Physics Divisions conducted a meta-analysis that included all of the Los Alamos and Livermore data, plus high-quality, independent data from other laboratories. Written up for the December 2010 issue of *Nuclear Data Sheets*, the meta-analysis showed that the results of the 1970s experiments are in excellent agreement with the best data known. Los Alamos and Livermore adjusted their conversion factors accordingly, and they once again agree on fission-yield estimates.

Though it took many years, the sister Laboratories turned what had become an entrenched scientific dispute into a fruitful and cooperative collaboration. And the final word from Barr? "It's about time."

—Jay Schecker

Better Fuel Cell Membrane Materials

Laboratory researchers Rangachary Mukundan, Melinda Einsla (now working at Rohm and Haas, a Dow Chemical subsidiary), and Fernando Garzon were impressed when Japanese scientists discovered a new material, tin pyrophosphate, that could potentially replace the proton-conducting polymer that formed the membrane in proton exchange membrane (PEM) fuel cells. The new low-cost, conductive ceramic material has a number of possible cost and performance advantages over the currently used fluorocarbon polymer membranes.

The membrane is central to PEM fuel cells, which produce electricity from hydrogen. At one end of the cell, a catalyst causes the hydrogen to split into protons and electrons, which are then routed along separate paths: the protons through the membrane (an electrolyte) and the electrons through an outside circuit as electrical current. At the cell's other end, the protons and electrons combine with oxygen to form water, the fuel cell's only emission.

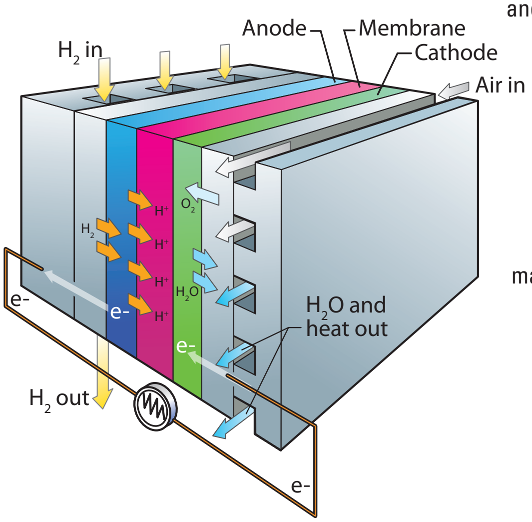
But there's a temperature problem. Current PEM fuel cells operate at 100 degrees Celsius and below, the temperature the polymer membrane needs to conduct protons. That relatively low temperature requires an expensive material, platinum, as the catalyst, making the fuel cell too expensive to be used in cars. In addition, it causes the water to form as a liquid rather than vapor. The liquid interferes with cell performance.

There are fuel cell technologies that use ceramic materials (other than tin pyrophosphate) that operate at greater than 700 degrees Celsius. Those allow for less-expensive catalysts and produce water in the form of vapor, but in cars the very high operational temperature would require exotic alloys and would make cold startup rather difficult and energy intensive.

The Japanese researchers found that the tin pyrophosphates could conduct protons at 200 to 300 degrees Celsius—hot enough to open the door for new catalysts and turn water to vapor but cool enough for common automobile materials. But the original way of making the new material had its own problems. The scientists were heating a mix of tin-containing oxide or salt with phosphoric acid to a molten state to evaporate off excess phosphorous oxides. That method produced the desired product, but the high heat left the product so nonuniform that only a small portion was usable. In addition, the process produced a very corrosive and acidic byproduct, phosphorous pentoxide.

The Los Alamos scientists found that they could start with different precursors—pyrophosphate salt and inorganic acid salt—dissolve them separately (several solvents worked, including water), mix them, and then evaporate out the solvent, this time at a lower temperature. The resulting product was a uniform tin pyrophosphate, and there were no corrosive byproducts. The newly patented process makes the synthesis of new membrane materials commercially possible.

—Eileen Patterson



A PEM fuel cell's membrane (magenta) is impermeable to electrons (e^-), forcing them to travel to through a wire to the cell's cathode (green), while the protons (hydrogen ions, H^+) go through the membrane. As shown in the figure, the protons and electrons separate when incoming hydrogen (H_2) encounters the catalyst mixed into the anode (blue). They meet again at the cathode, where a catalyst causes them to combine with oxygen (O_2) to form water.

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